

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
 Data File : BM043727.D
 Acq On : 03 Jan 2024 11:31
 Operator : MA/JU
 Sample : 05919-14RE
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 GCF46RE

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.828	105	109	120	rBV	95315	280538	0.18%	0.067%
2	4.081	137	152	172	rBV	323839	1183953	0.74%	0.283%
3	4.499	220	223	237	rVB4	53695	160023	0.10%	0.038%
4	5.040	309	315	325	rVB3	131569	262156	0.16%	0.063%
5	5.457	370	386	393	rBV	168539	414403	0.26%	0.099%
6	5.675	416	423	431	rBV	2060484	3223796	2.03%	0.769%
7	5.752	431	436	442	rVV2	162575	319903	0.20%	0.076%
8	6.022	476	482	488	rBV	135755	281463	0.18%	0.067%
9	6.075	488	491	506	rVB2	70350	182398	0.11%	0.044%
10	6.246	511	520	530	rVB	1083920	1634163	1.03%	0.390%
11	6.475	550	559	570	rBV7	150240	471482	0.30%	0.113%
12	6.863	615	625	633	rBV2	171459	364054	0.23%	0.087%
13	7.016	644	651	656	rVV2	196378	485006	0.30%	0.116%
14	7.151	664	674	691	rVB	391667	901595	0.57%	0.215%
15	7.304	691	700	712	rBV2	336862	797283	0.50%	0.190%
16	7.422	712	720	725	rVV3	75958	183037	0.12%	0.044%
17	7.498	725	733	741	rVB	413658	737791	0.46%	0.176%
18	7.598	741	750	756	rBV	461106	789877	0.50%	0.188%
19	7.722	763	771	782	rVB6	118580	347077	0.22%	0.083%
20	7.963	806	812	817	rBV	1327202	2112872	1.33%	0.504%
21	8.040	817	825	837	rBV	17770333	31208984	19.61%	7.448%
22	8.181	845	849	853	rBV2	108904	176982	0.11%	0.042%
23	8.581	910	917	926	rVB3	134488	302042	0.19%	0.072%
24	8.693	930	936	943	rBV	478014	796136	0.50%	0.190%
25	8.763	943	948	954	rVV	222226	362647	0.23%	0.087%
26	9.140	1005	1012	1016	rBV	401473	689428	0.43%	0.165%
27	9.175	1016	1018	1028	rVB	147898	211867	0.13%	0.051%
28	9.292	1030	1038	1045	rBV	394409	843310	0.53%	0.201%
29	9.487	1064	1071	1076	rBV4	296644	662236	0.42%	0.158%
30	9.545	1076	1081	1093	rVB5	269975	672248	0.42%	0.160%
31	9.792	1118	1123	1128	rBV	307323	510114	0.32%	0.122%
32	9.857	1128	1134	1142	rVV	328144	614794	0.39%	0.147%
33	10.081	1167	1172	1177	rVV4	335961	654366	0.41%	0.156%
34	10.292	1202	1208	1222	rBV	1319006	2730790	1.72%	0.652%
35	10.410	1223	1228	1234	rVB	413701	755433	0.47%	0.180%
36	10.534	1245	1249	1255	rVB5	105816	186679	0.12%	0.045%

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37	10.734	1275	1283	1288	rBV	12532149	22312955	14.02%	5.325%
38	10.828	1296	1299	1303	rVV2	342797	421488	0.26%	0.101%
39	10.869	1303	1306	1311	rVB3	174937	252923	0.16%	0.060%
40	11.004	1321	1329	1334	rBV	2514984	4694645	2.95%	1.120%
41	11.098	1339	1345	1350	rBV2	3364718	5953977	3.74%	1.421%
42	11.281	1372	1376	1385	rVB2	736840	1378196	0.87%	0.329%
43	11.375	1386	1392	1409	rVB	5060818	10609755	6.67%	2.532%
44	11.598	1425	1430	1435	rBV5	308916	745579	0.47%	0.178%
45	11.675	1440	1443	1452	rVB4	369817	738885	0.46%	0.176%
46	11.775	1456	1460	1462	rBV	488766	715140	0.45%	0.171%
47	12.028	1499	1503	1516	rVB3	810970	1617788	1.02%	0.386%
48	12.181	1522	1529	1533	rBV	3576907	7447399	4.68%	1.777%
49	12.433	1568	1572	1586	rVB	1797367	3321039	2.09%	0.793%
50	12.651	1606	1609	1624	rVB	1010509	2003162	1.26%	0.478%
51	12.839	1631	1641	1651	rBV4	2094251	9804362	6.16%	2.340%
52	12.992	1663	1667	1677	rVB2	1053612	2565626	1.61%	0.612%
53	13.075	1678	1681	1685	rVV2	986177	1738888	1.09%	0.415%
54	13.128	1686	1690	1707	rVB	2252620	5597472	3.52%	1.336%
55	13.422	1734	1740	1752	rBV	10936699	31423795	19.74%	7.499%
56	13.792	1796	1803	1813	rBV2	2019496	7316977	4.60%	1.746%
57	13.951	1822	1830	1833	rBV3	3686461	10936446	6.87%	2.610%
58	14.075	1848	1851	1856	rBV2	2843327	6008327	3.78%	1.434%
59	14.516	1918	1926	1965	rBV4	20389532	159149585	100.00%	37.980%
60	14.839	1976	1981	1994	rBV	7586333	27823318	17.48%	6.640%
61	19.868	2834	2836	2837	rBV	5912332	5781625	3.63%	1.380%
62	20.386	2921	2924	2925	rBV2	6540868	7678316	4.82%	1.832%
63	20.898	3002	3011	3013	rBV9	7361978	24489042	15.39%	5.844%

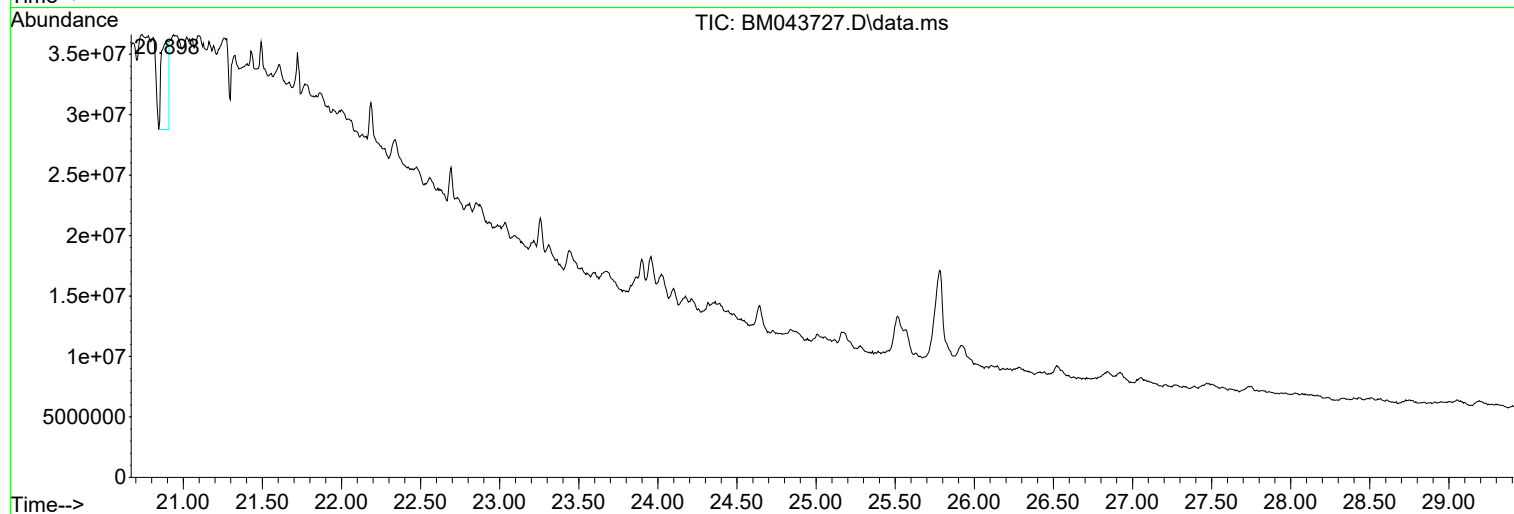
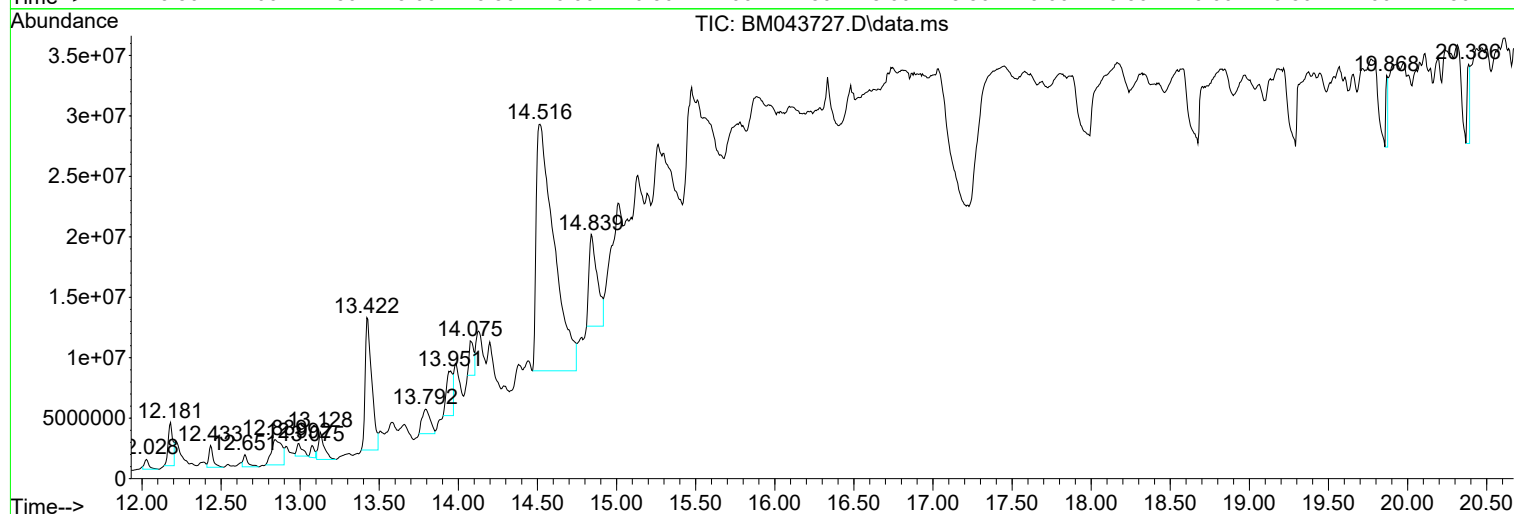
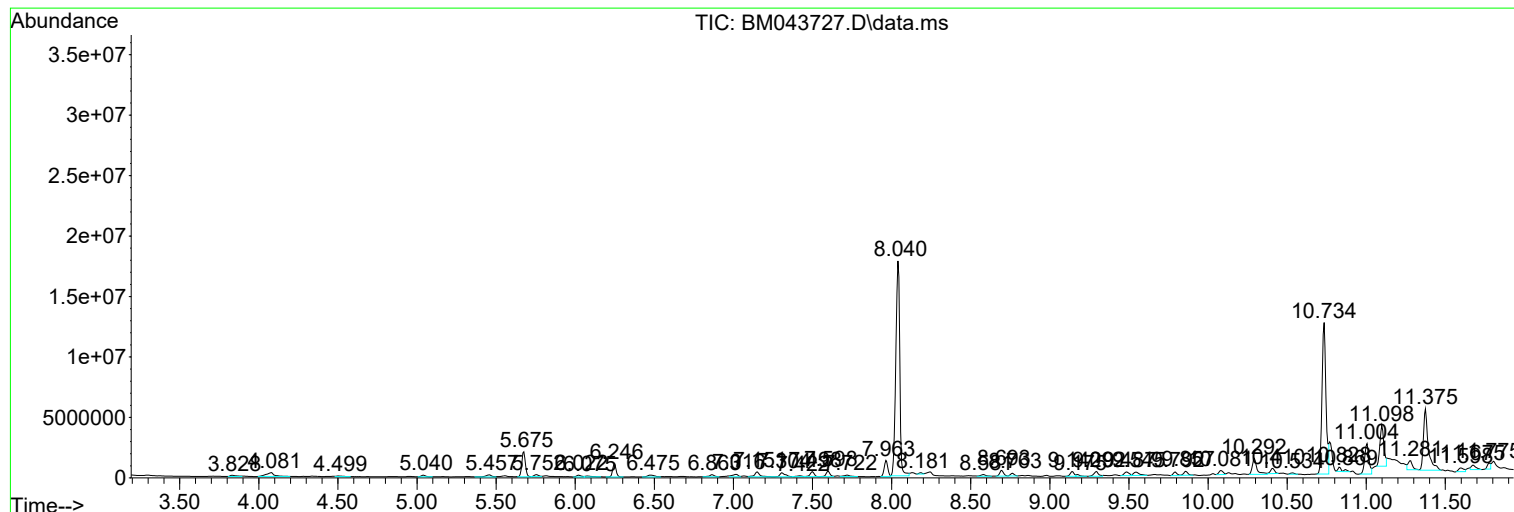
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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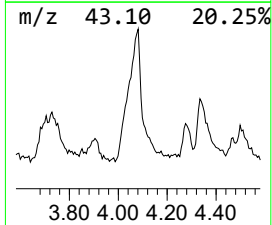
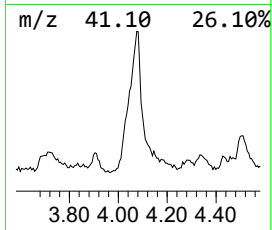
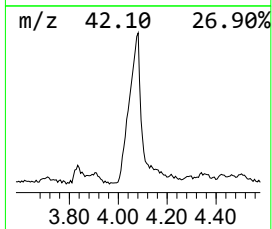
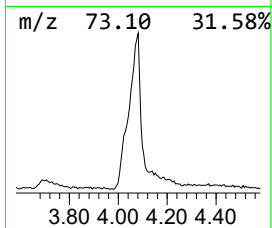
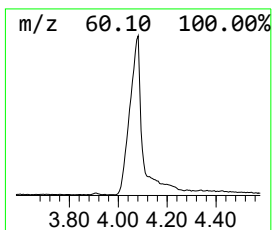
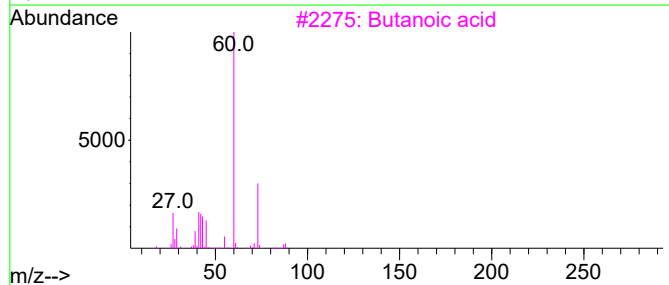
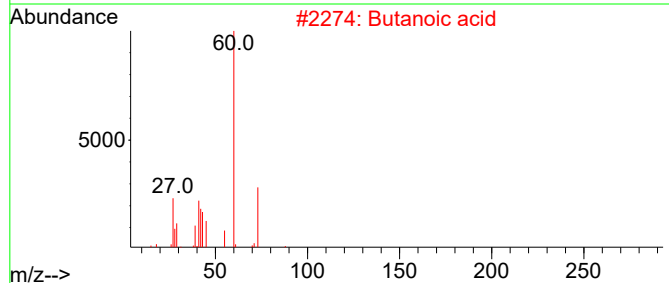
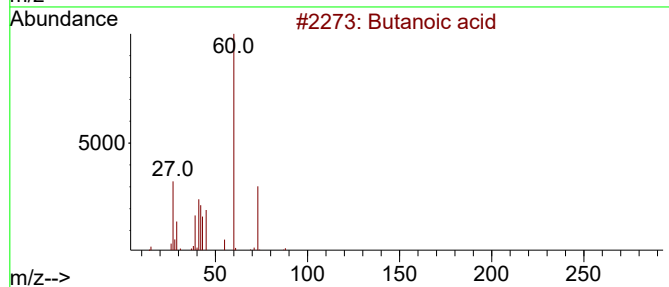
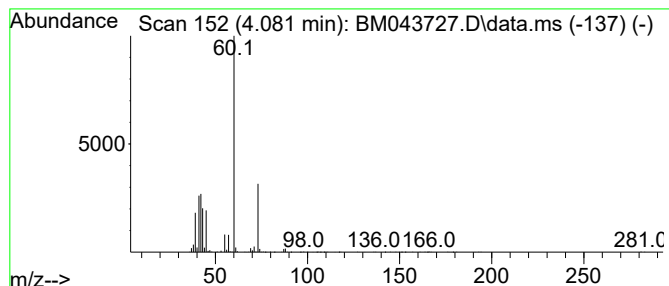
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.081	11.21 ng/ul	1183950	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Butanoic acid	88	C4H8O2	000107-92-6	72
3			Butanoic acid	88	C4H8O2	000107-92-6	64
4			Butanoic acid	88	C4H8O2	000107-92-6	59
5			Hexanoic acid	116	C6H12O2	000142-62-1	40



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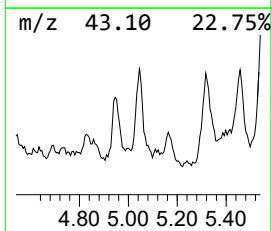
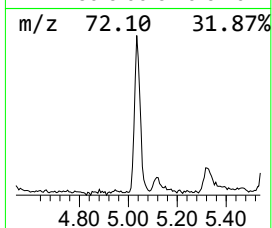
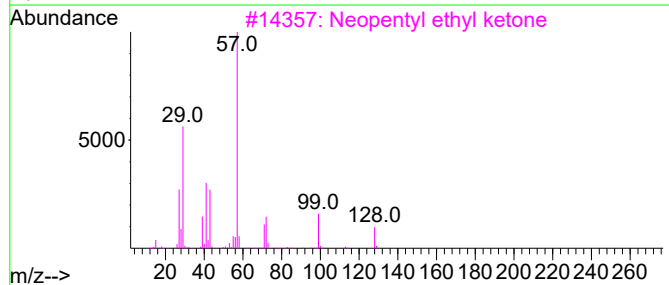
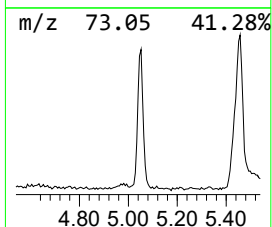
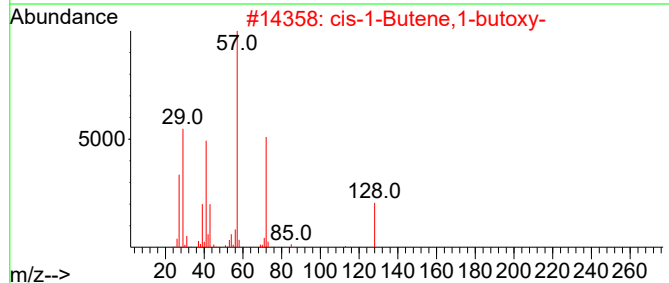
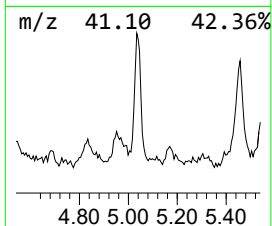
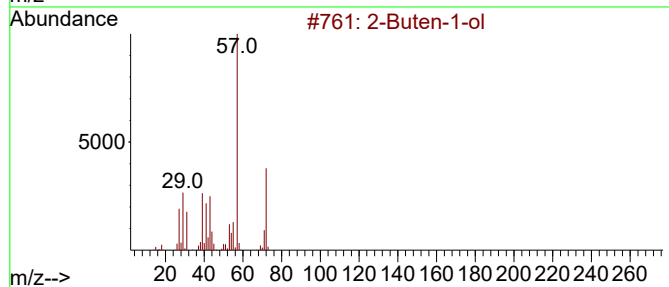
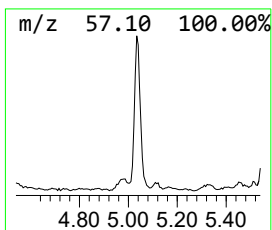
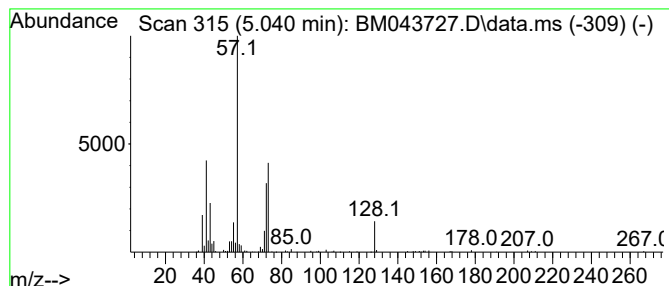
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.48 ng/ul	262156	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Buten-1-ol	72	C4H8O	006117-91-5	49
2			cis-1-Butene,1-butoxy-	128	C8H16O	1000139-52-7	47
3			Neopentyl ethyl ketone	128	C8H16O	005340-30-7	47
4			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	47
5			2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	40



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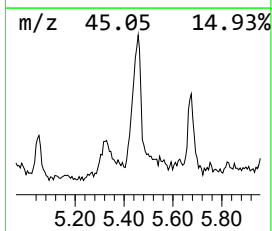
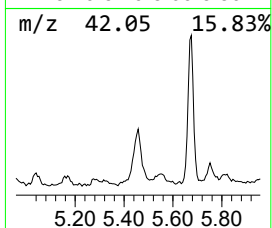
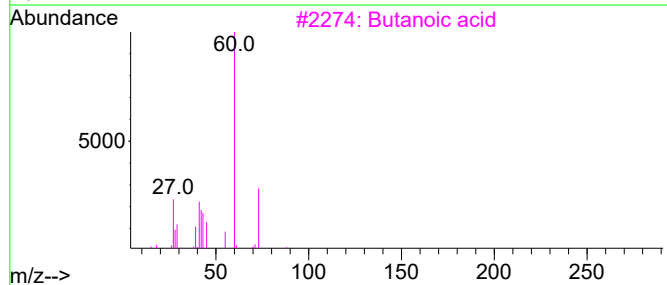
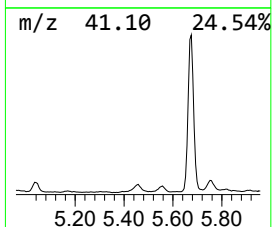
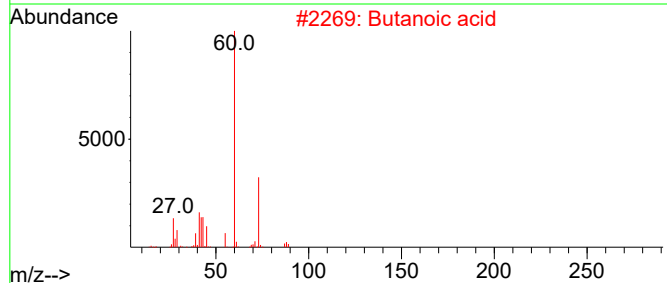
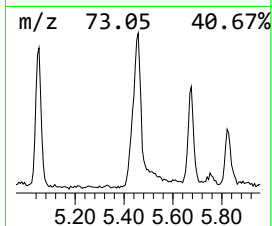
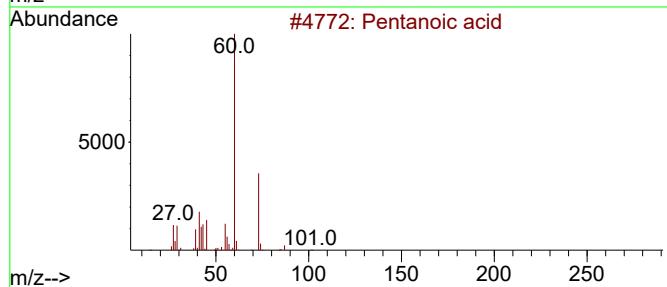
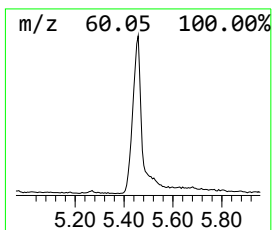
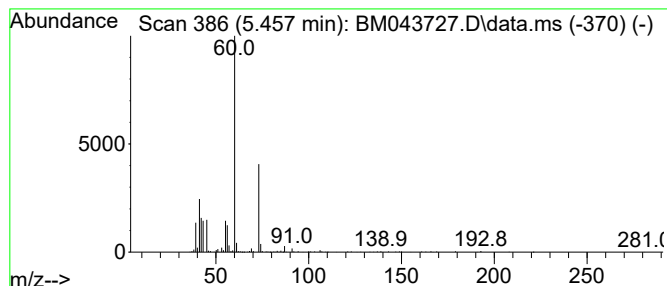
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.457	3.92 ng/ul	414403	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	83
2			Butanoic acid	88	C4H8O2	000107-92-6	78
3			Butanoic acid	88	C4H8O2	000107-92-6	72
4			Butanoic acid	88	C4H8O2	000107-92-6	72
5			Butanoic acid	88	C4H8O2	000107-92-6	64



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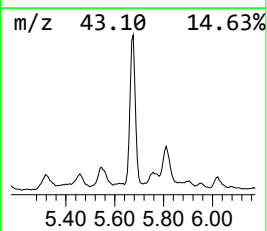
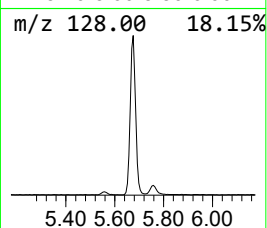
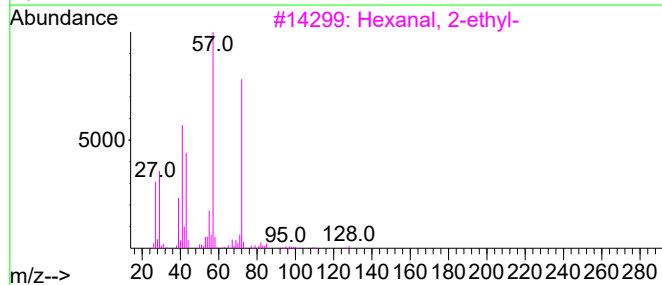
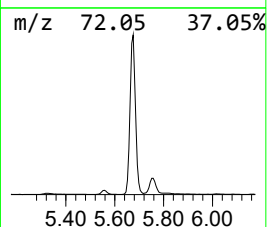
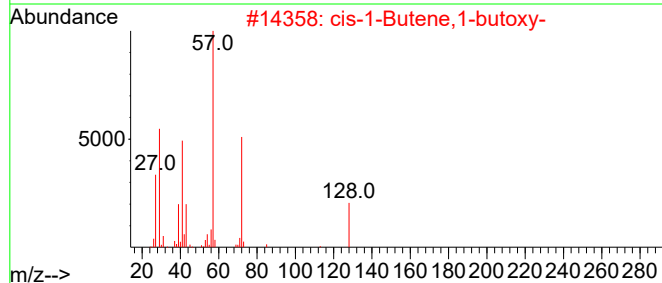
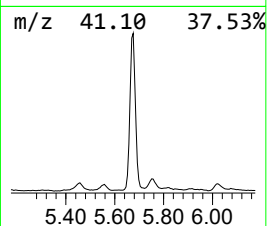
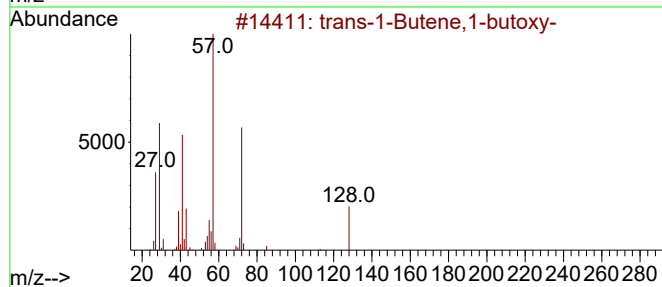
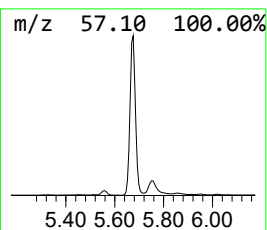
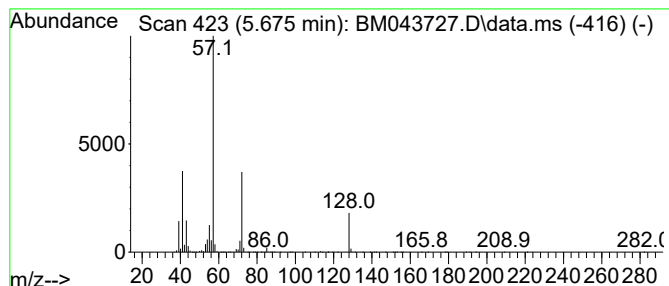
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 trans-1-Butene,1-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.675	30.52 ng/ul	3223800	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	74
2			cis-1-Butene,1-butoxy-	128	C8H16O	1000139-52-7	64
3			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	50
4			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	47
5			3-Methyl-3-oxetanemethanol	102	C5H10O2	003143-02-0	45



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ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF46RE

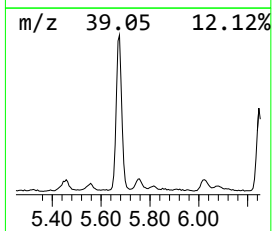
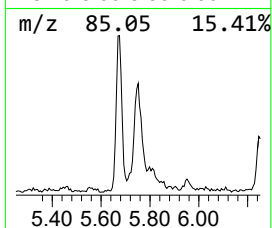
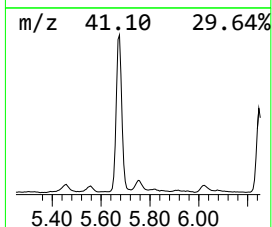
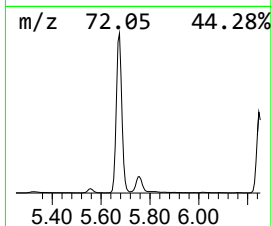
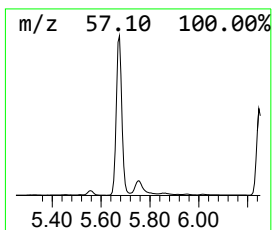
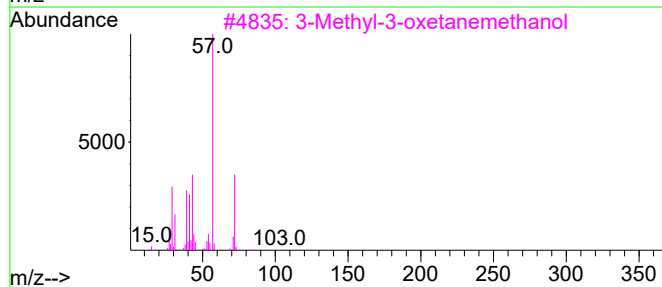
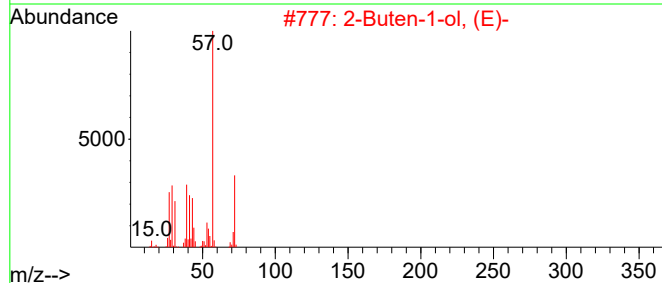
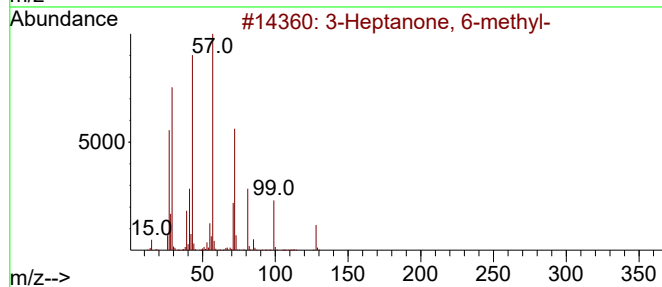
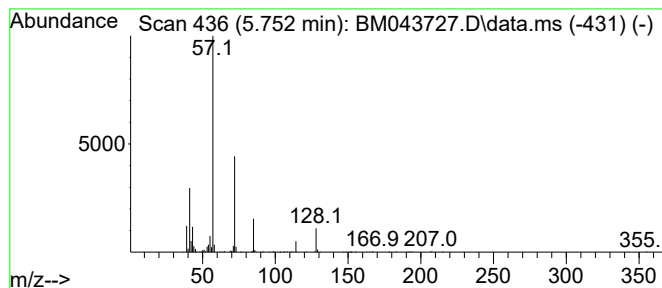
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Heptanone, 6-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.752	3.03 ng/ul	319903	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	64
2			2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	40
3			3-Methyl-3-oxetanemethanol	102	C5H10O2	003143-02-0	40
4			2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	40
5			Hexanal, 2,2-dimethyl-	128	C8H16O	000996-12-3	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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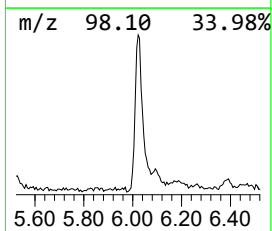
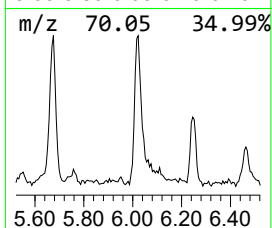
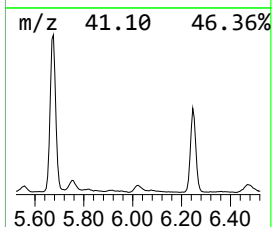
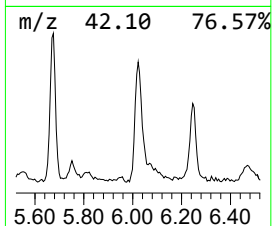
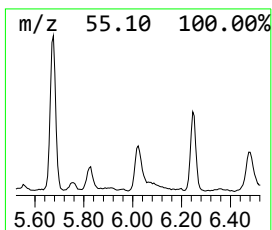
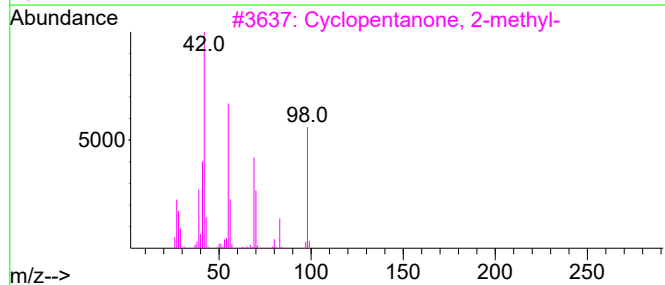
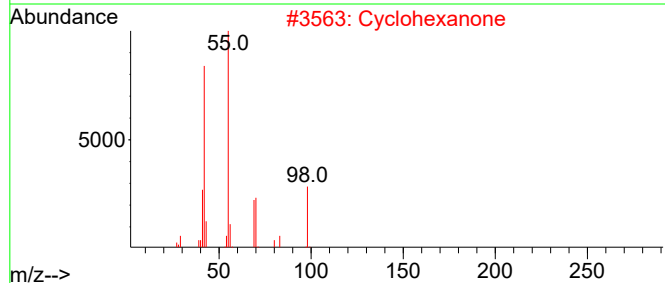
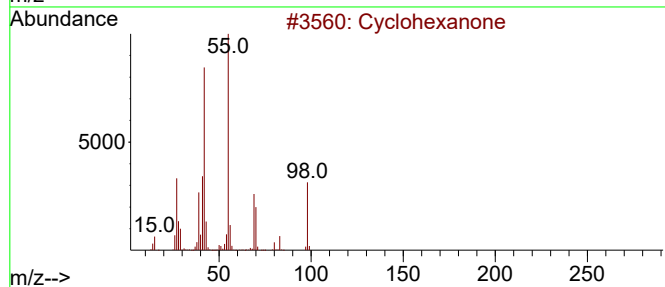
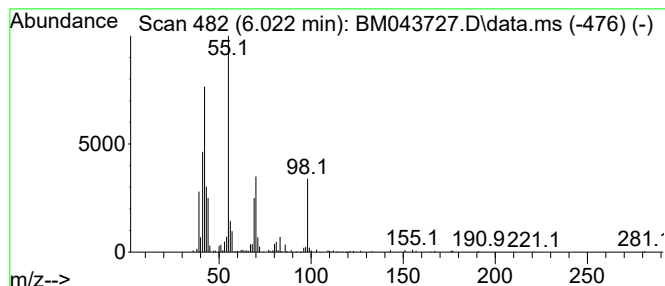
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexanone Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.022	2.66 ng/ul	281463	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	76
2			Cyclohexanone	98	C6H10O	000108-94-1	72
3			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	52
4			Cyclohexanone	98	C6H10O	000108-94-1	46
5			Cyclohexanone	98	C6H10O	000108-94-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
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Sample : 05919-14RE
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Instrument :
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ClientSampleId :
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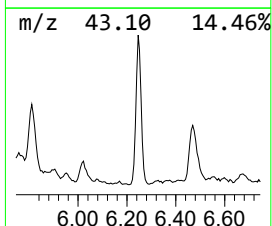
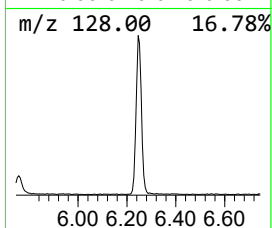
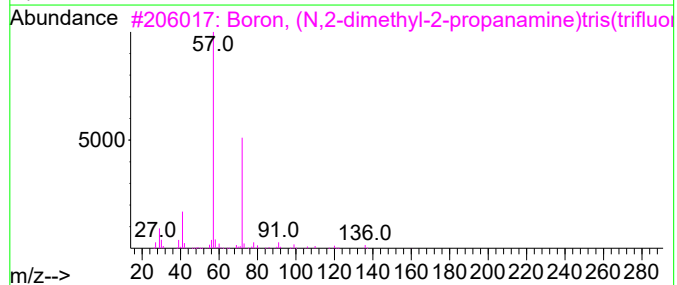
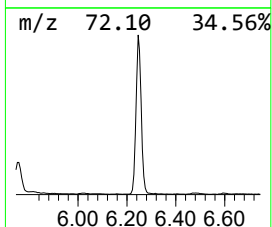
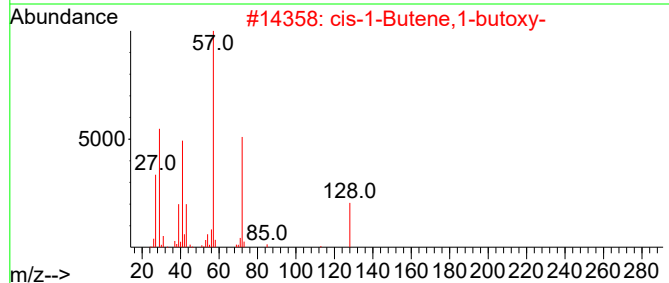
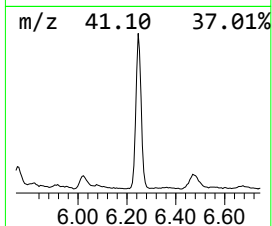
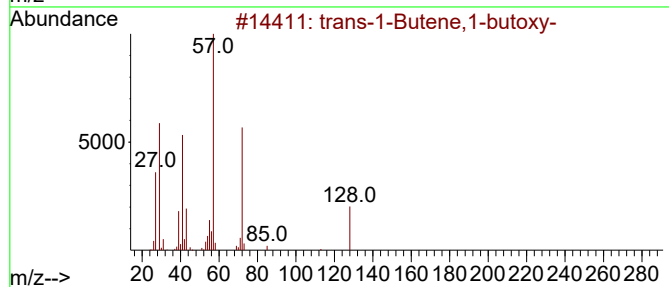
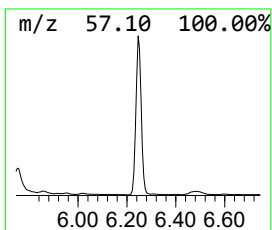
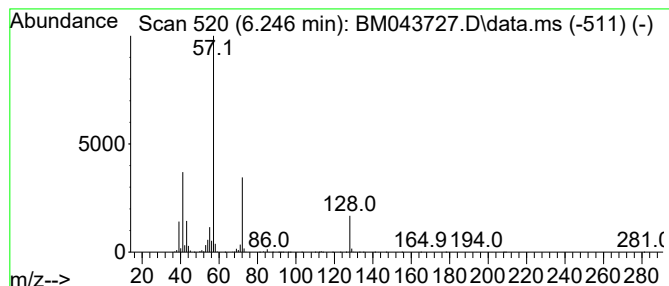
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 cis-1-Butene,1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.246	15.47 ng/ul	1634160	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	64
2			cis-1-Butene,1-butoxy-	128	C8H16O	1000139-52-7	50
3			Boron, (N,2-dimethyl-2-propanami...	305	C8H13BF9N	128353-59-3	40
4			2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	37
5			3-Methyl-3-oxetanemethanol	102	C5H10O2	003143-02-0	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
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Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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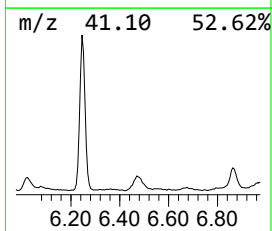
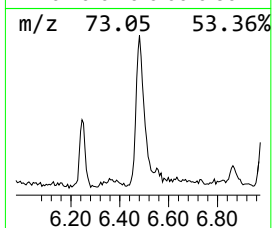
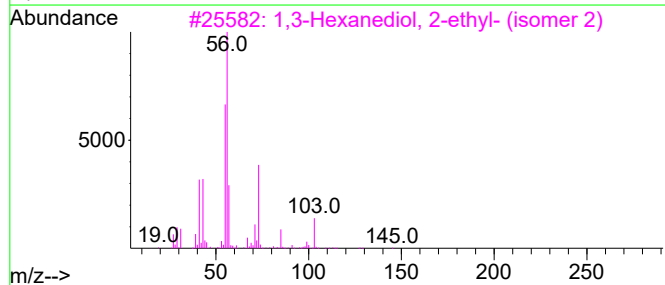
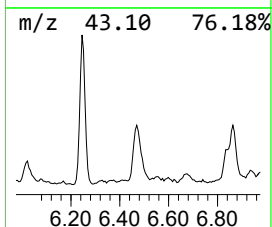
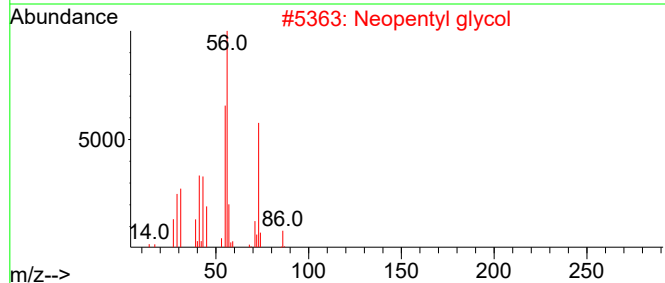
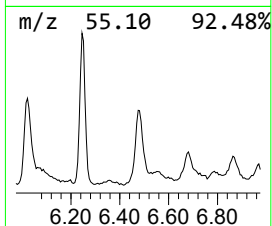
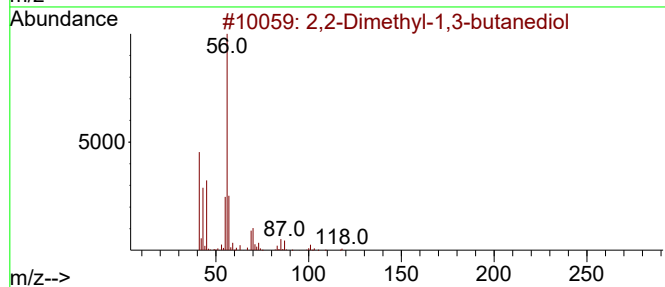
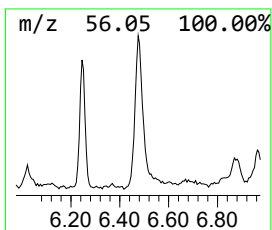
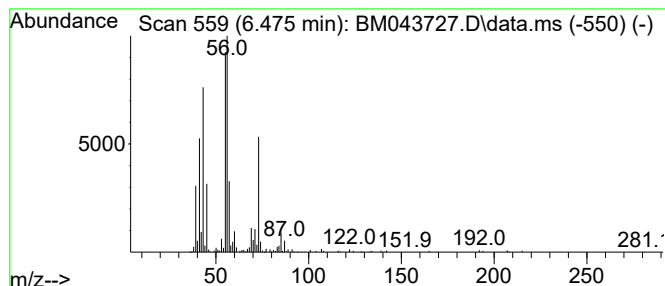
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2,2-Dimethyl-1,3-butanediol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	4.46 ng/ul	471482	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	59
2			Neopentyl glycol	104	C5H12O2	000126-30-7	50
3			1,3-Hexanediol, 2-ethyl- (isomer 2)	146	C8H18O2	1000484-18-1	50
4			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	43
5			Neopentyl glycol	104	C5H12O2	000126-30-7	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
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Misc :
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Instrument :
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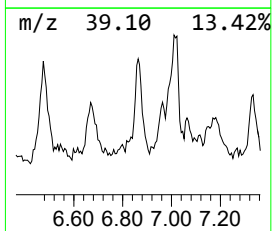
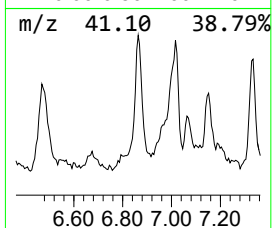
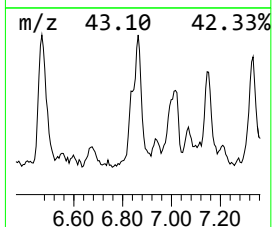
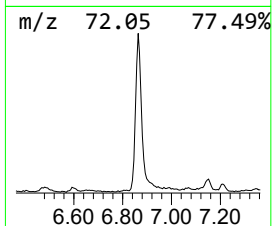
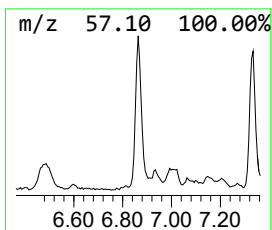
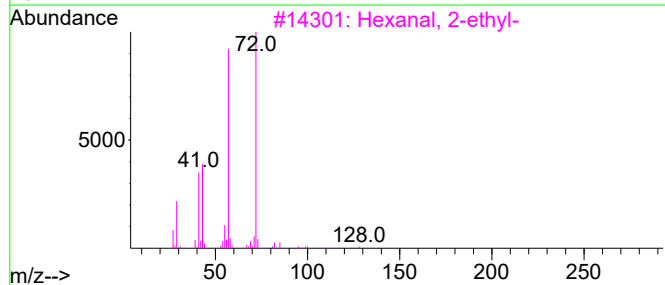
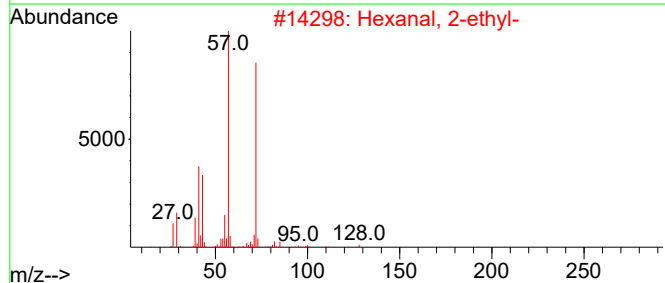
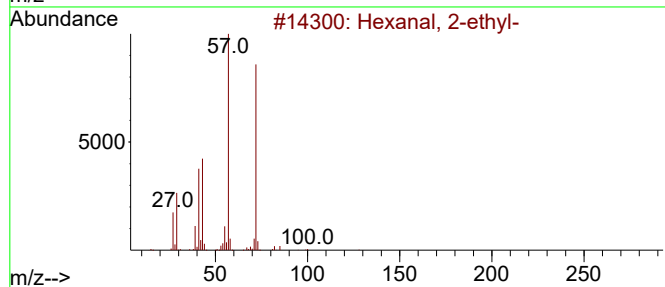
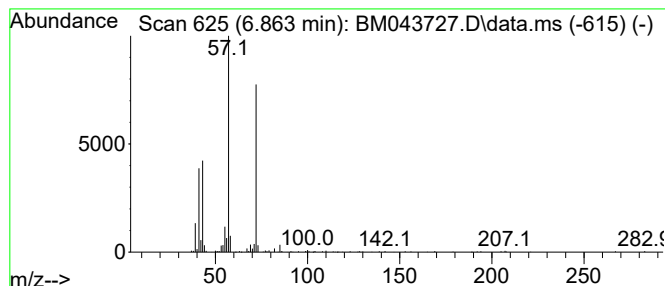
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hexanal, 2-ethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.863	3.45 ng/ul	364054	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	83
2			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	56
3			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	56
4			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	56
5			2-(dimethylamino)-1-(2-methoxyph...	207	C12H17NO2	1000456-74-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
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Acq On : 03 Jan 2024 11:31
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Instrument :
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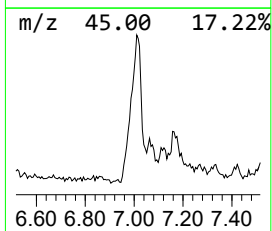
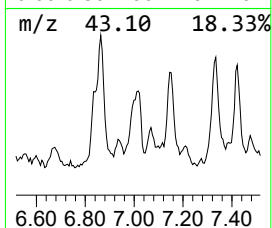
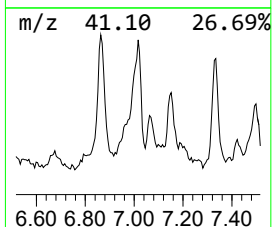
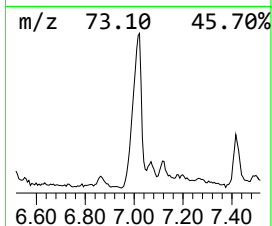
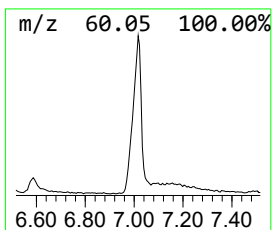
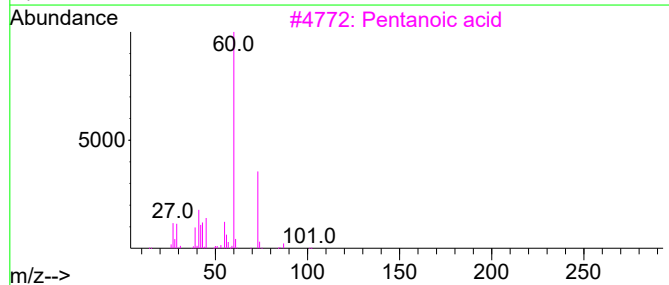
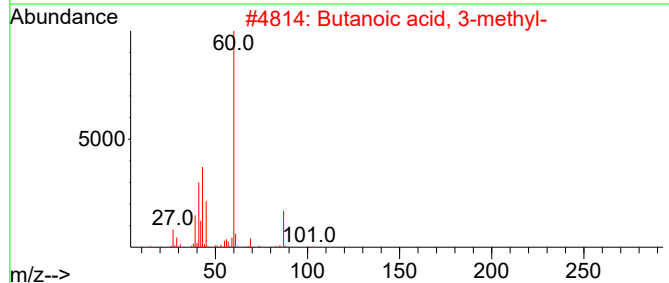
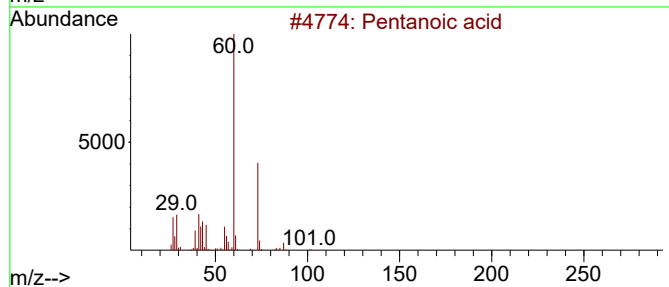
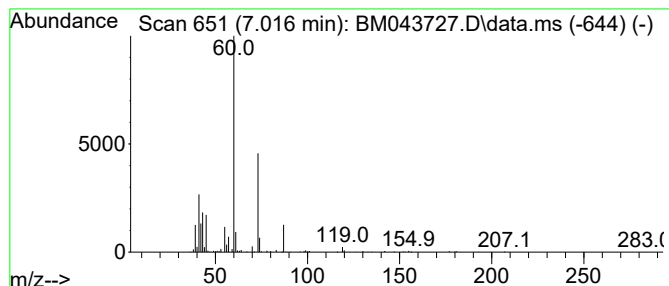
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Butanoic acid, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.016	4.59 ng/ul	485006	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	83
2			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
3			Pentanoic acid	102	C5H10O2	000109-52-4	72
4			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
5			Octanoic acid	144	C8H16O2	000124-07-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
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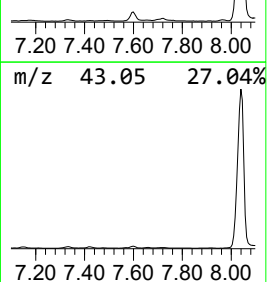
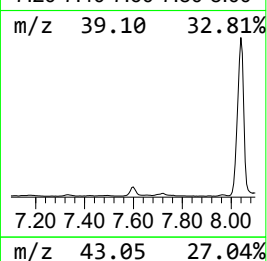
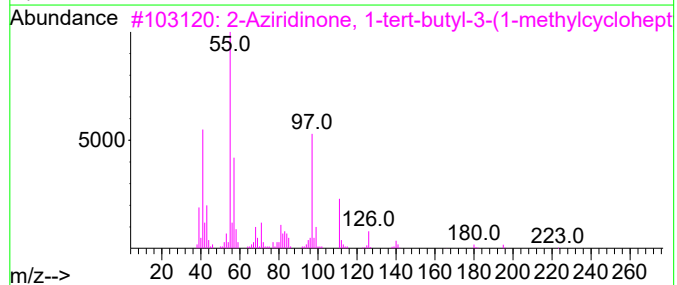
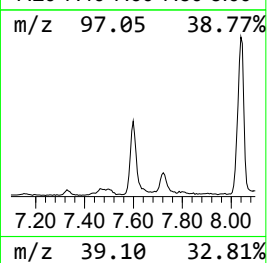
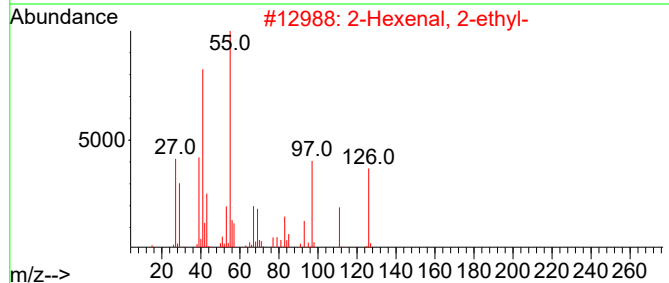
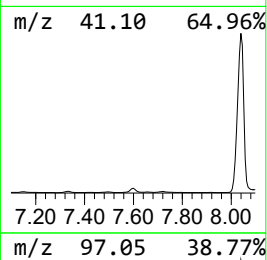
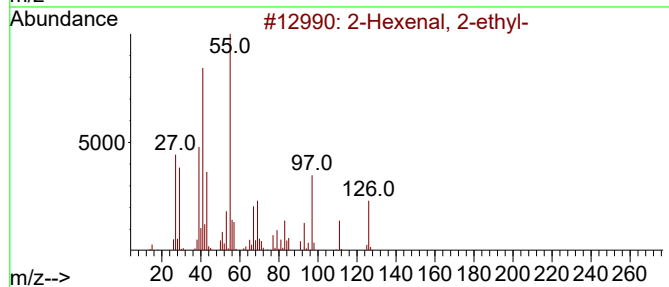
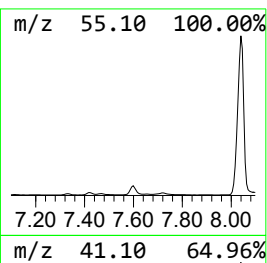
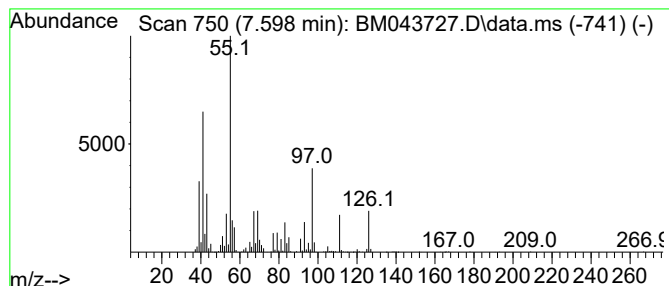
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2-Hexenal, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD			R.T.
7.598	7.48 ng/ul	789877	1,4-Dichlorobenzene-d4			7.963
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Hexenal, 2-ethyl-		126	C8H14O	000645-62-5	93
2	2-Hexenal, 2-ethyl-		126	C8H14O	000645-62-5	68
3	2-Aziridinone, 1-tert-butyl-3-(1...		223	C14H25NO	026944-18-3	53
4	2-Hexenal, 2-ethyl-		126	C8H14O	000645-62-5	53
5	Cyclopentane, 1-methyl-2-propyl-		126	C9H18	003728-57-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
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Instrument :
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ClientSampleId :
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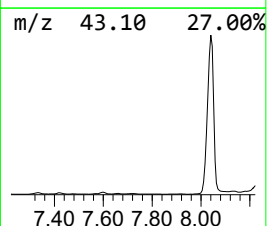
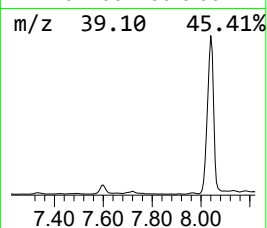
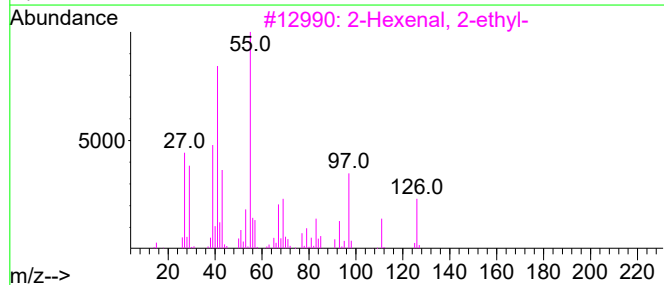
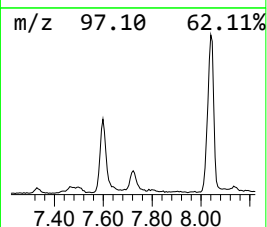
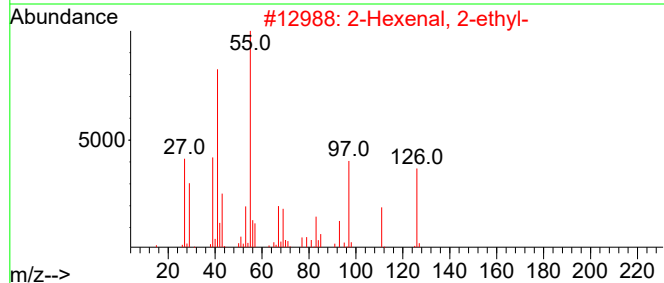
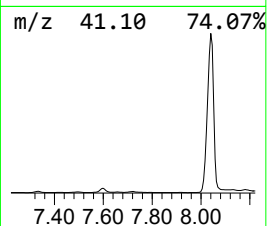
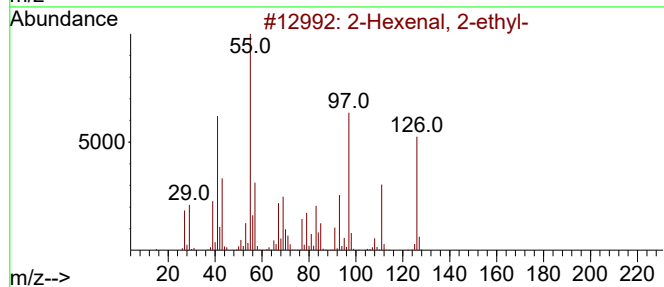
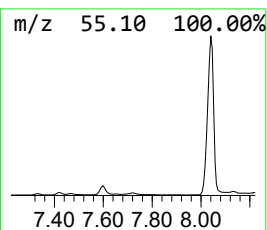
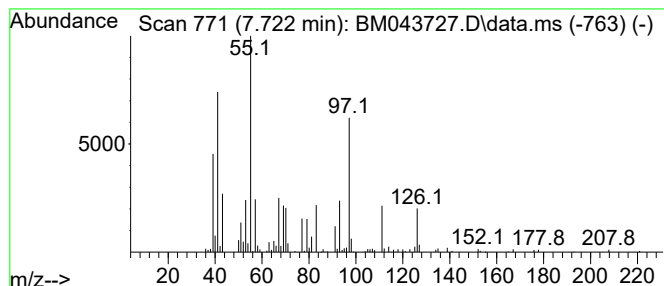
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown-02 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	3.29 ng/ul	347077	1,4-Dichlorobenzene-d4	7.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	64	
2	2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	53	
3	2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	50	
4	4,4-Dimethyl-cyclohex-2-en-1-ol	126	C8H14O	1010143-72-5	49	
5	7-Oxabicyclo[4.1.0]heptan-2-one,...	126	C7H10O2	021889-89-4	38	



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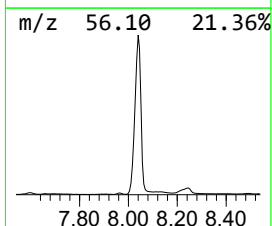
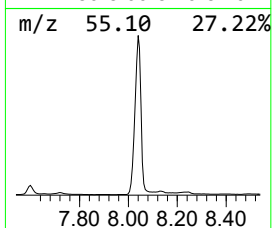
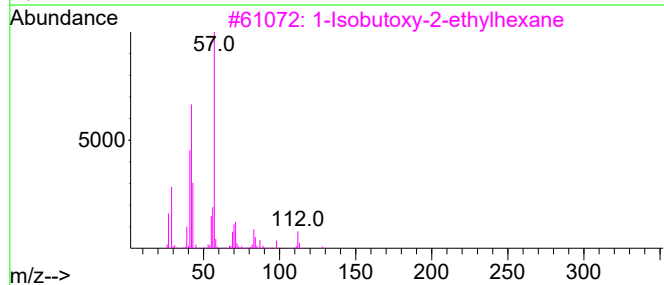
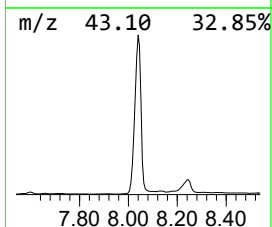
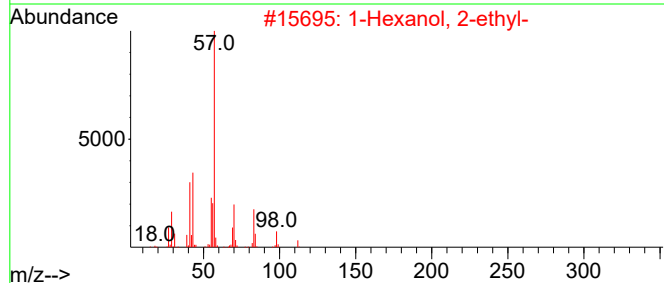
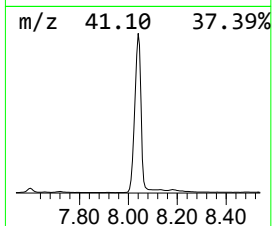
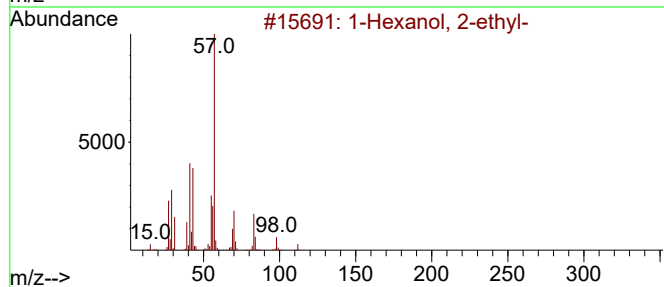
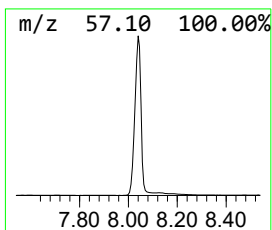
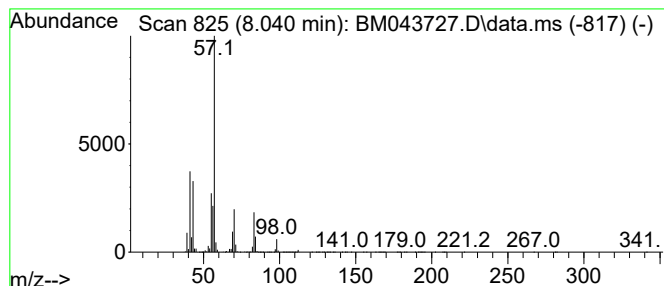
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.040	295.42 ng/ul	31209000	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Isobutoxy-2-ethylhexane			186	C12H26O	1000139-90-3	64
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
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ClientSampleId :
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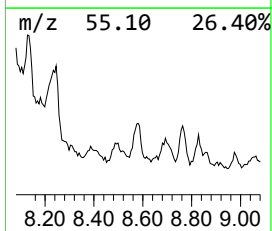
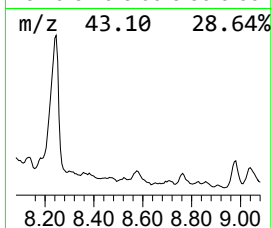
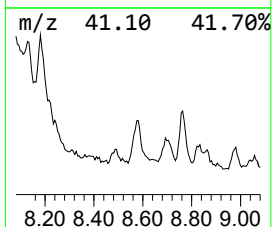
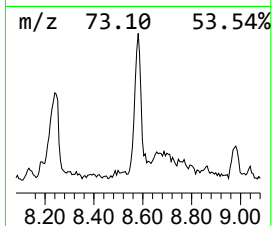
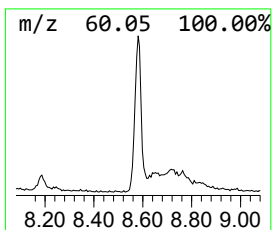
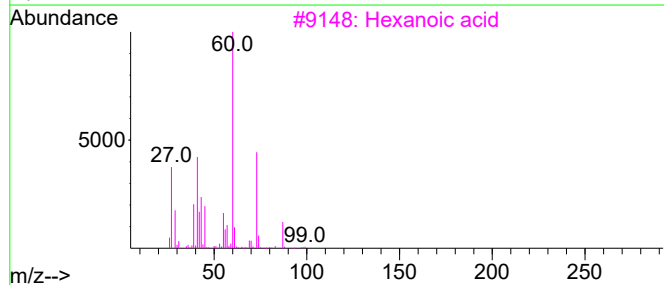
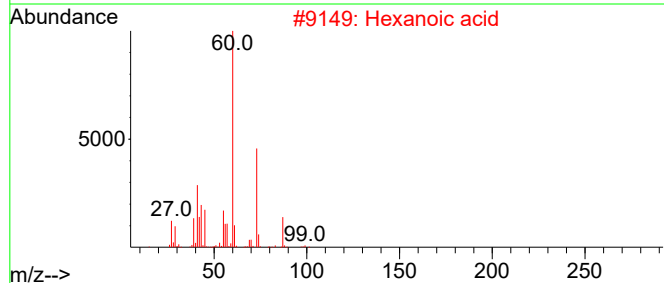
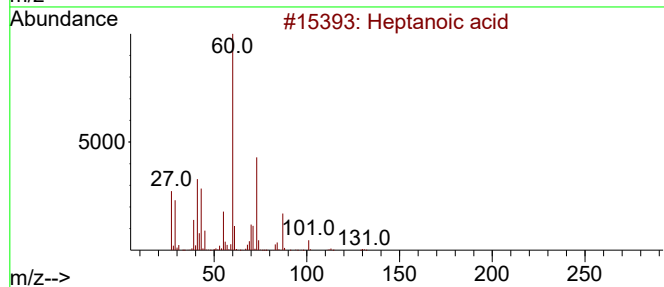
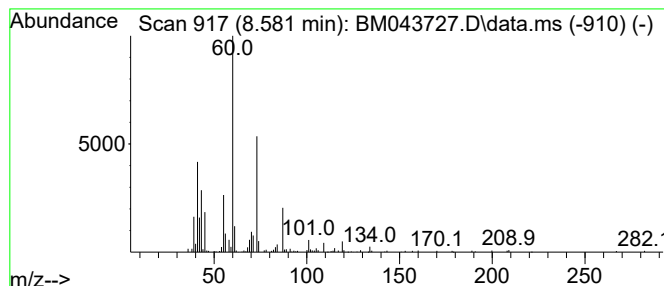
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heptanoic acid Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	2.86 ng/ul	302042	1,4-Dichlorobenzene-d4	7.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptanoic acid	130	C7H14O2	000111-14-8	78
2		Hexanoic acid	116	C6H12O2	000142-62-1	72
3		Hexanoic acid	116	C6H12O2	000142-62-1	59
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
5		Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	019467-01-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
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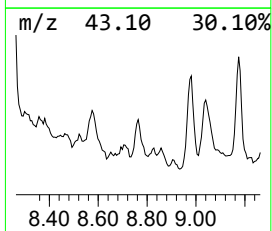
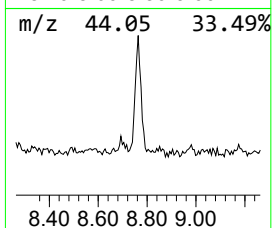
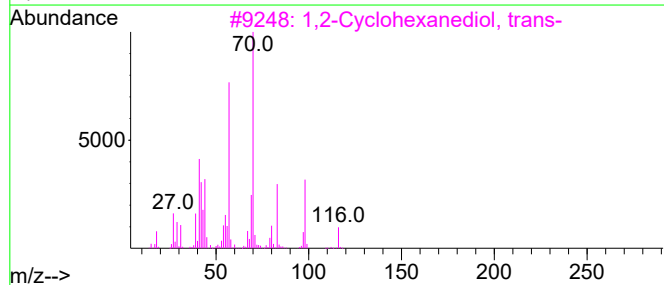
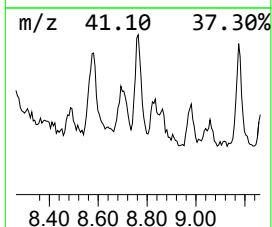
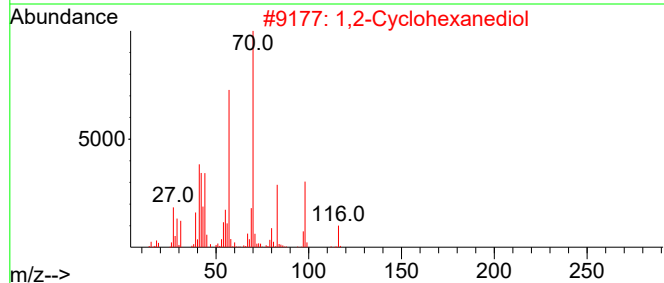
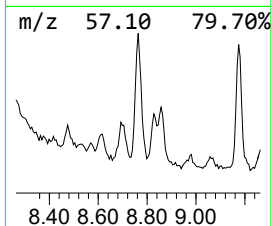
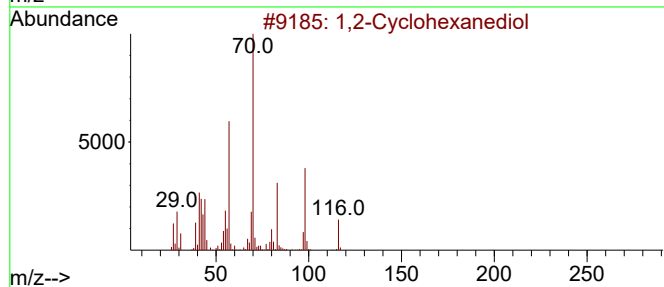
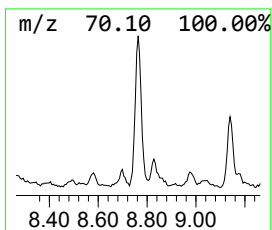
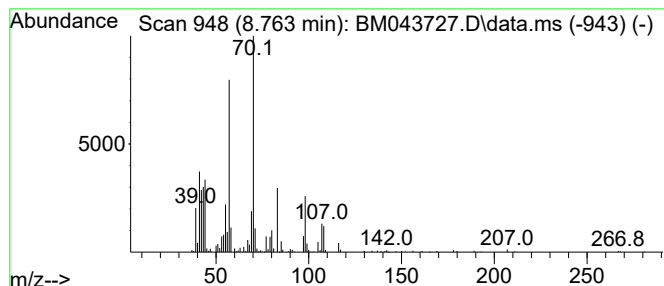
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1,2-Cyclohexanediol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.763	3.43 ng/ul	362647	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Cyclohexanediol	116	C6H12O2	000931-17-9	93
2			1,2-Cyclohexanediol	116	C6H12O2	000931-17-9	90
3			1,2-Cyclohexanediol, trans-	116	C6H12O2	001460-57-7	90
4			1,2-Cyclohexanediol	116	C6H12O2	000931-17-9	87
5			cis-1,2-Cyclohexanediol	116	C6H12O2	001792-81-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
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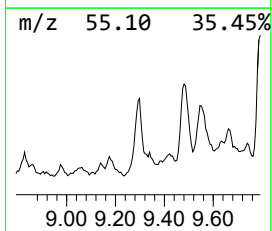
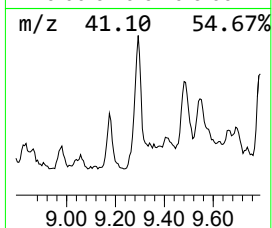
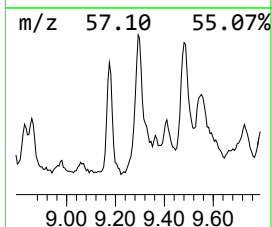
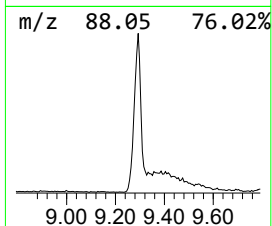
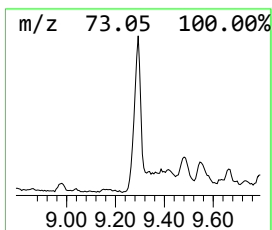
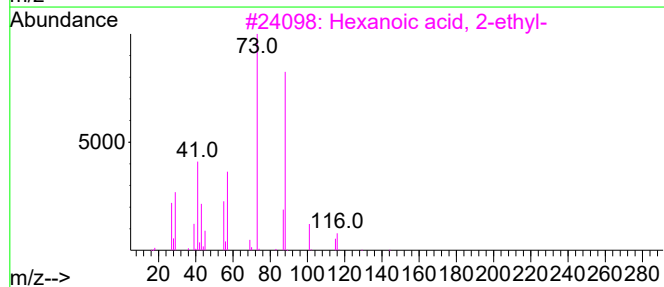
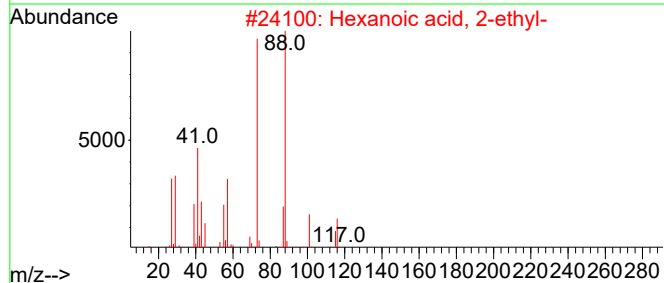
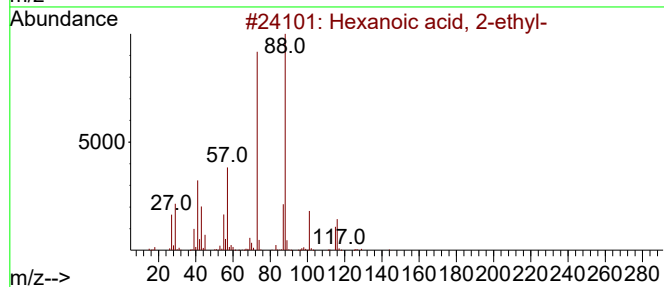
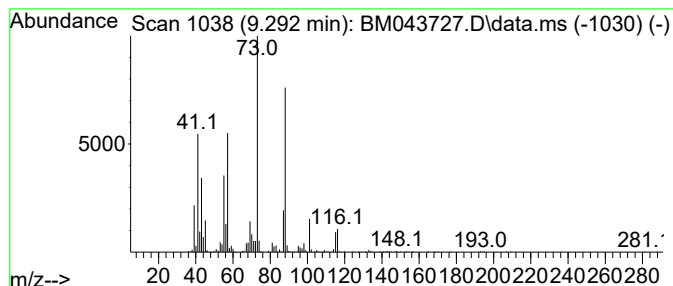
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.292	7.98 ng/ul	843310	1,4-Dichlorobenzene-d4	7.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
4			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
5			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	59



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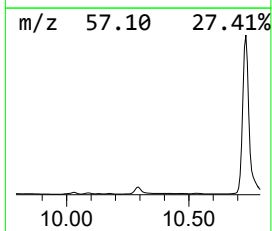
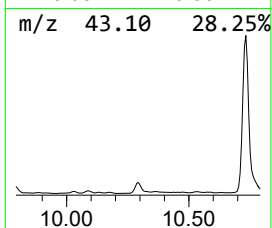
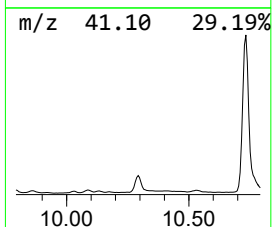
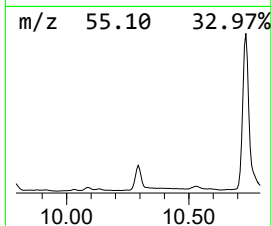
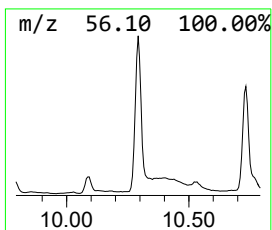
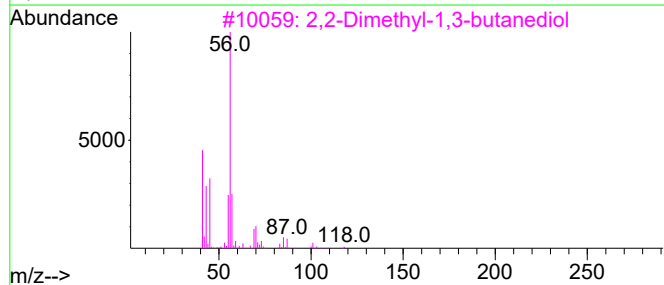
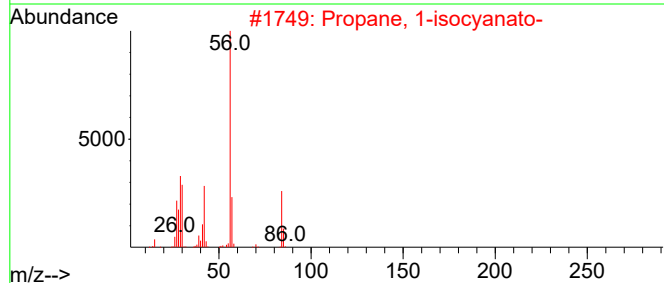
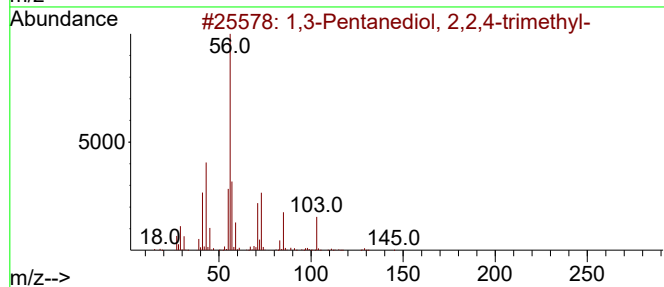
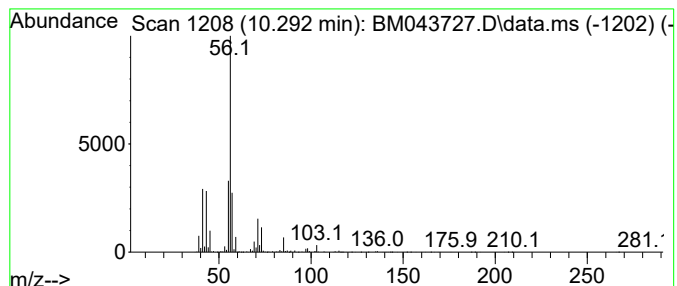
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.292	2.45 ng/ul	2730790	Naphthalene-d8	10.775	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50
2	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
3	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	38
4	Cyclobutane, 1,2,3,4-tetramethyl-	112	C8H16	069531-57-3	28
5	Cyclohexylamine	99	C6H13N	000108-91-8	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
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ALS Vial : 41 Sample Multiplier: 1

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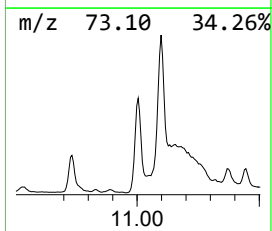
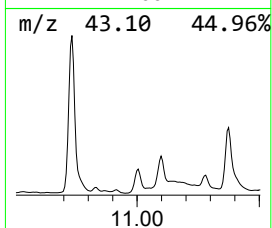
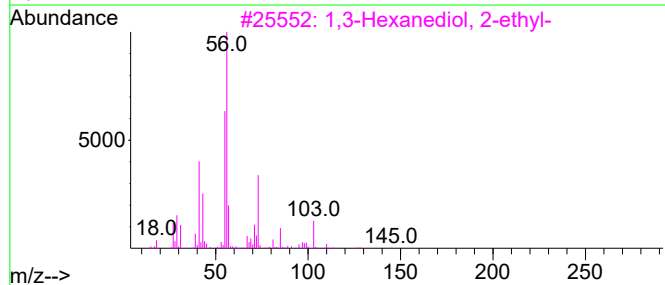
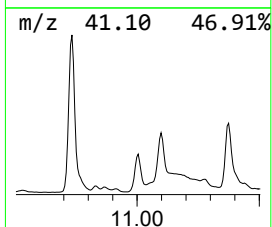
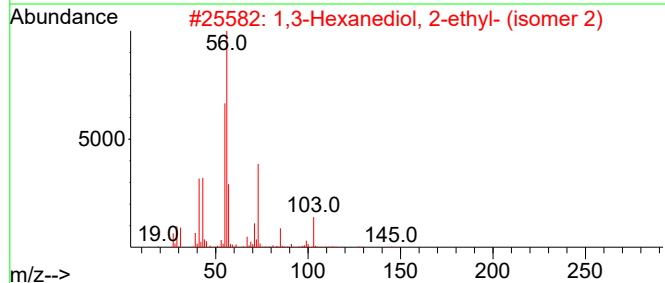
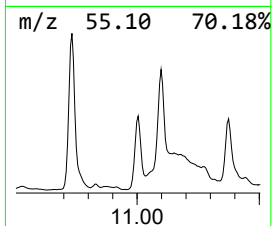
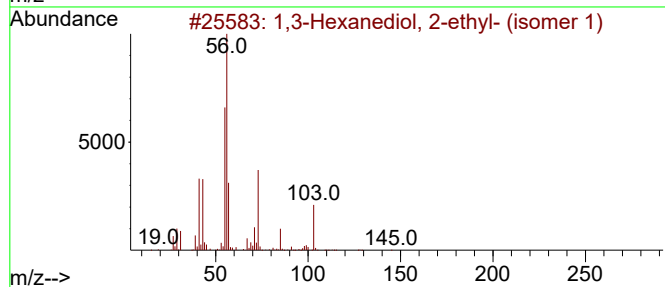
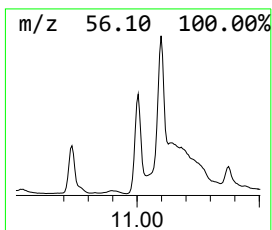
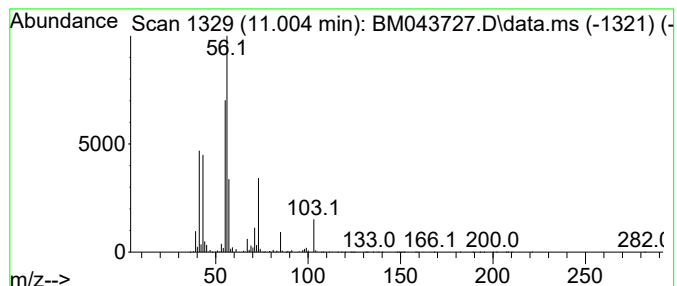
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 1,3-Hexanediol, 2-ethyl- (i... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.004	4.21 ng/ul	4694650	Naphthalene-d8	10.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	90		
2	1,3-Hexanediol, 2-ethyl- (isomer 2)	146	C8H18O2	1000484-18-1	83		
3	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	64		
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	47		
5	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

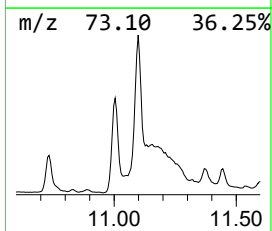
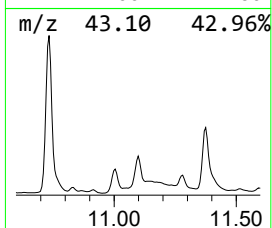
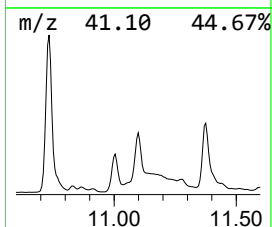
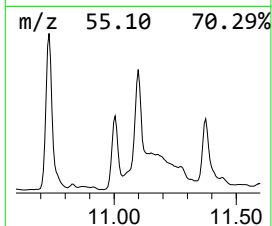
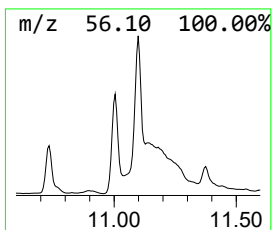
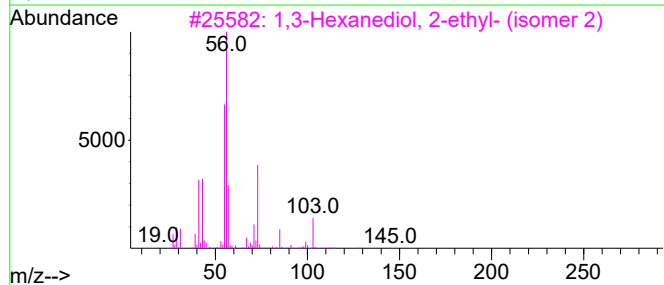
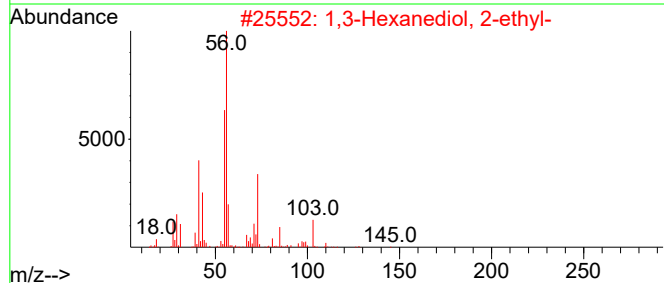
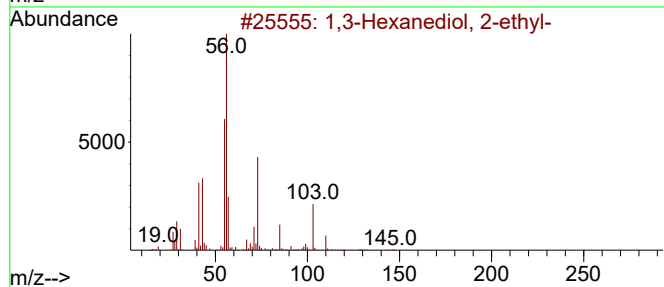
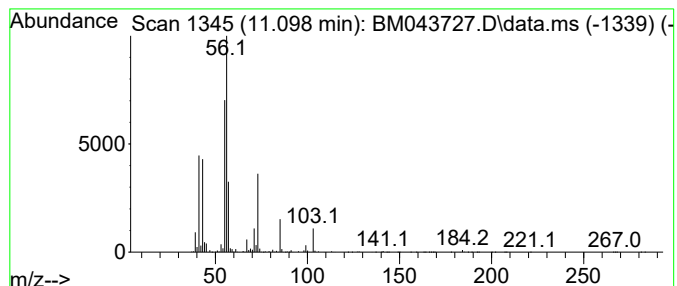
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 1,3-Hexanediol, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.098	5.34 ng/ul	5953980	Naphthalene-d8	10.775	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	83
2	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	83
3	1,3-Hexanediol, 2-ethyl- (isomer 2)	146	C8H18O2	1000484-18-1	78
4	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	64
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF46RE

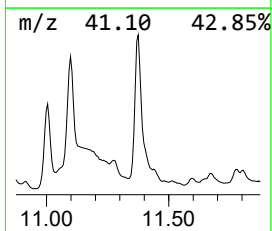
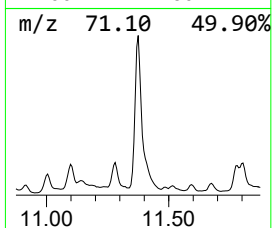
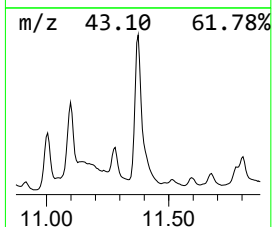
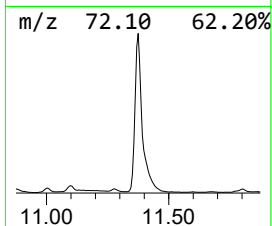
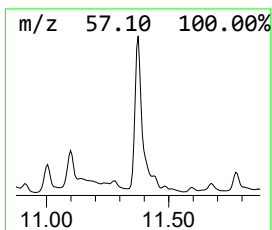
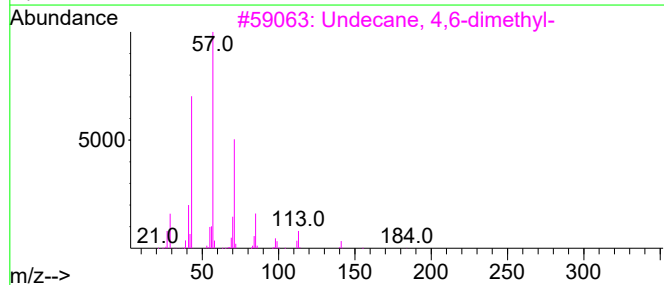
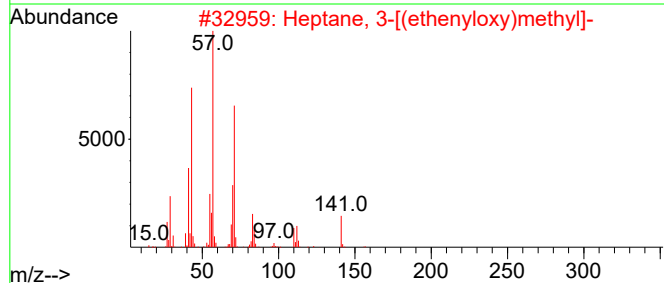
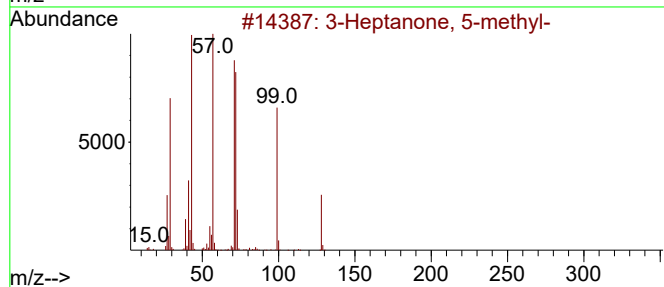
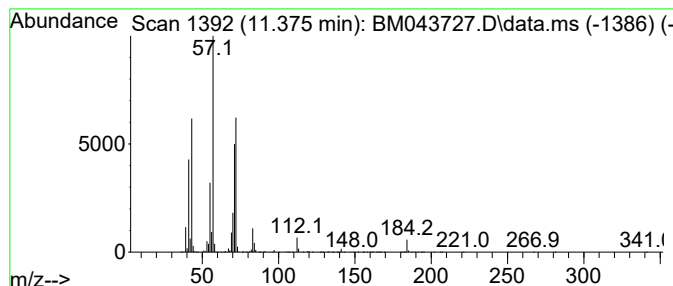
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 3-Heptanone, 5-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.375	9.51 ng/ul	10609800	Naphthalene-d8	10.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	50
2		Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	50
3		Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	50
4		Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	50
5		Undecane, 6-ethyl-	184	C13H28	017312-60-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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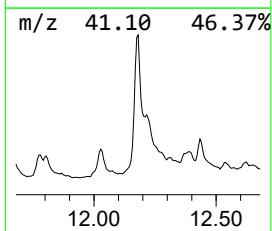
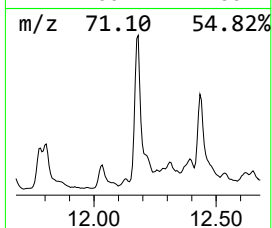
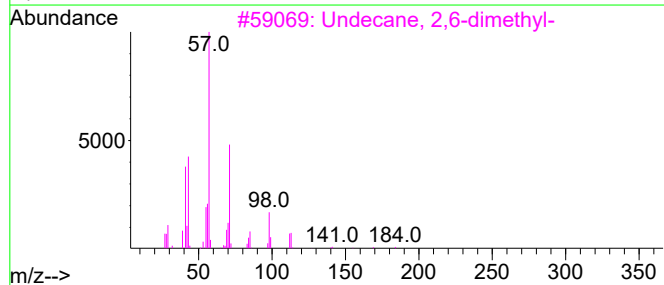
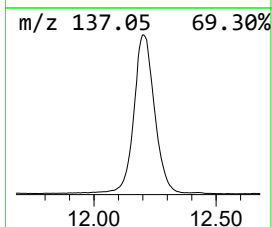
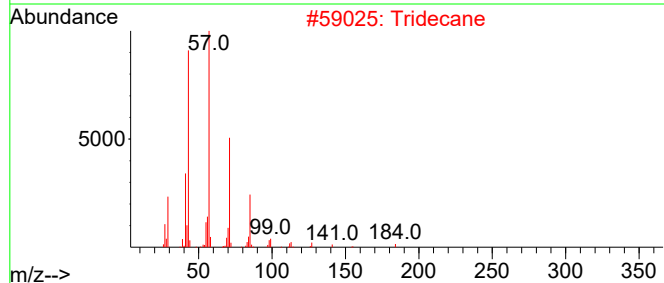
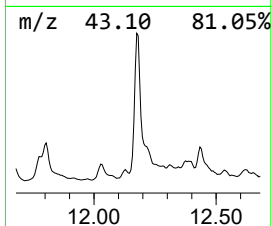
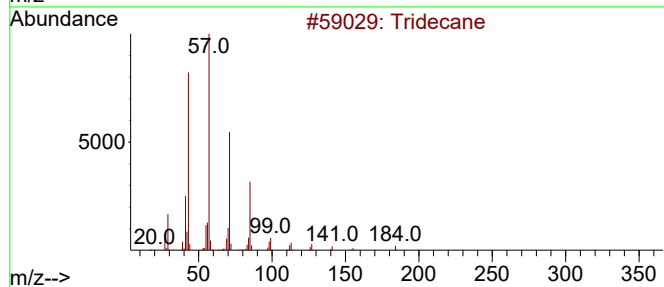
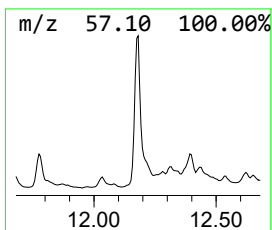
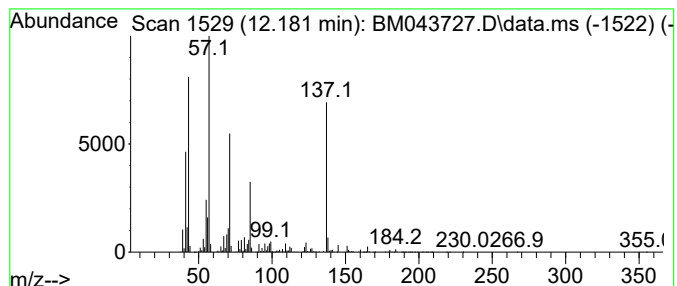
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 21 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.181	6.68 ng/ul	7447400	Naphthalene-d8	10.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	60
2			Tridecane	184	C13H28	000629-50-5	60
3			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	50
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	49
5			Hexadecane	226	C16H34	000544-76-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

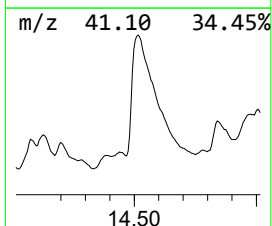
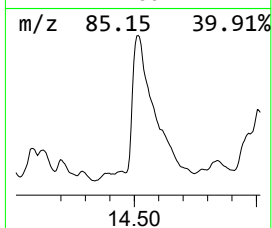
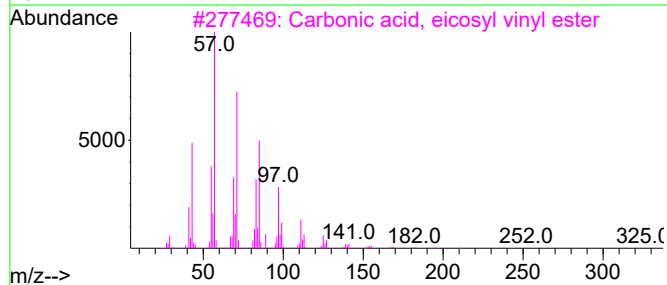
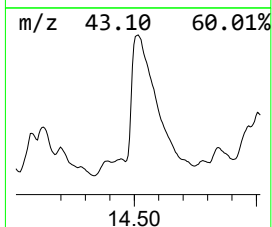
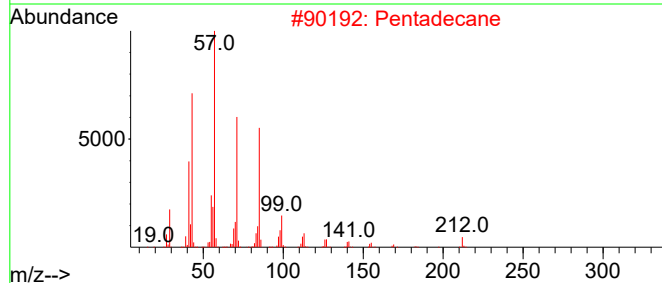
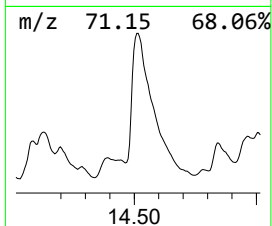
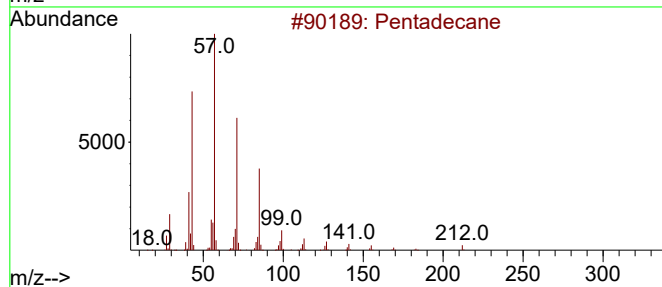
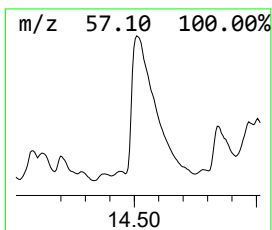
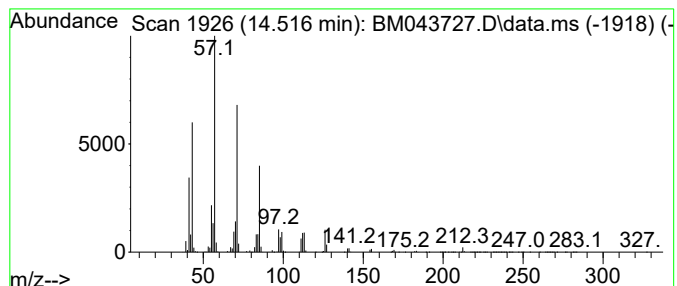
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 22 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.516	20.00 ng/ul	159150000	Acenaphthene-d10	14.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Pentadecane	212	C15H32	000629-62-9	87
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
4	Tridecane	184	C13H28	000629-50-5	80
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF46RE

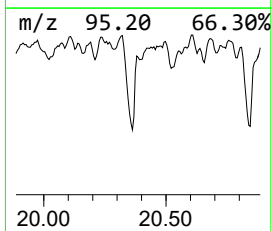
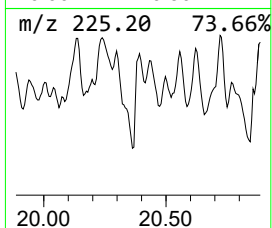
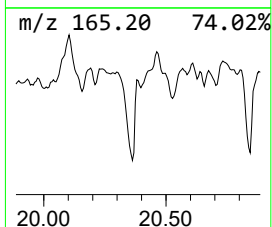
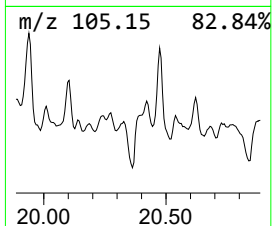
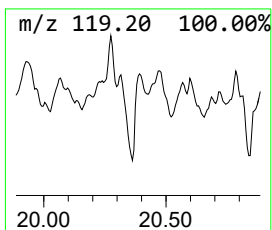
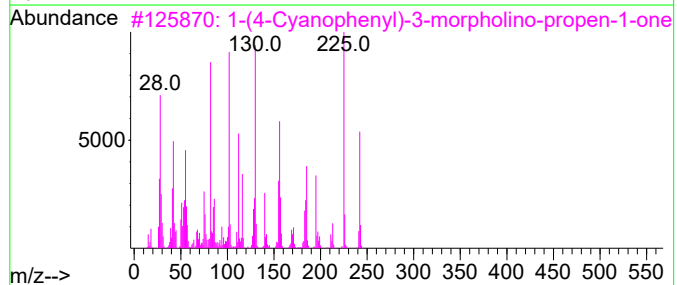
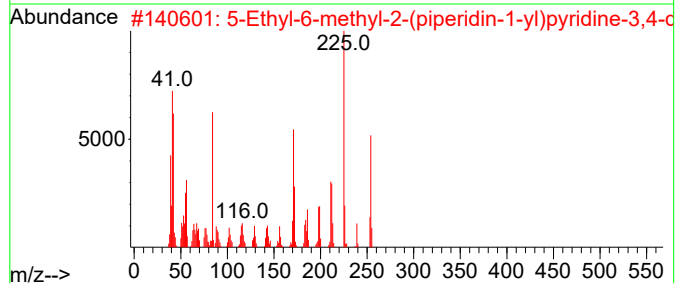
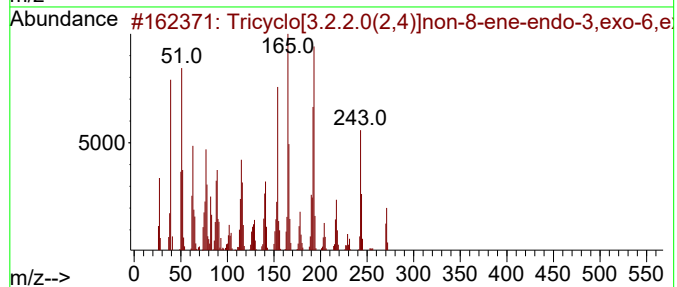
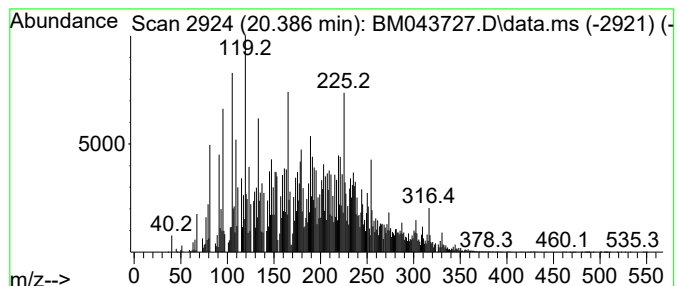
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 23 Tricyclo[3.2.2.0(2,4)]non-8... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.386	6.27 ng/ul	7678320	Chrysene-d12	21.609

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[3.2.2.0(2,4)]non-8-ene-...	271	C18H13N3	1000154-27-8	90
2			5-Ethyl-6-methyl-2-(piperidin-1-...	254	C15H18N4	1000409-47-6	35
3			1-(4-Cyanophenyl)-3-morpholino-p...	242	C14H14N2O2	153495-93-3	25
4			Benzo[b]1,4-dioxane-2-carboxylic...	210	C10H10O5	102575-15-5	25
5			Isoquinoline, 1,2,3,4-tetrahydro...	251	C17H17NO	349094-27-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043727.D
Acq On : 03 Jan 2024 11:31
Operator : MA/JU
Sample : 05919-14RE
Misc :
ALS Vial : 41 Sample Multiplier: 1

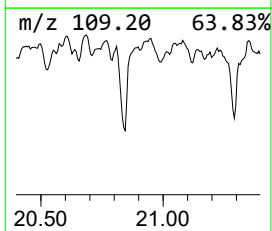
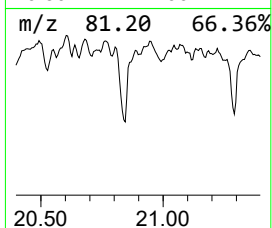
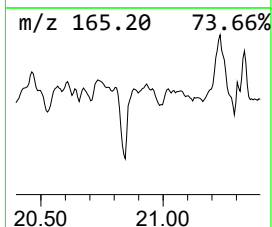
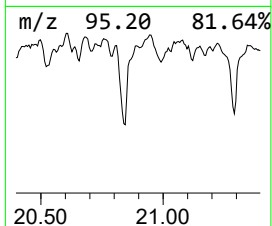
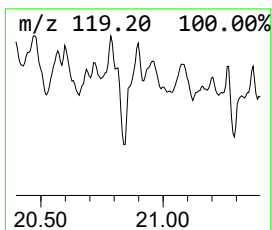
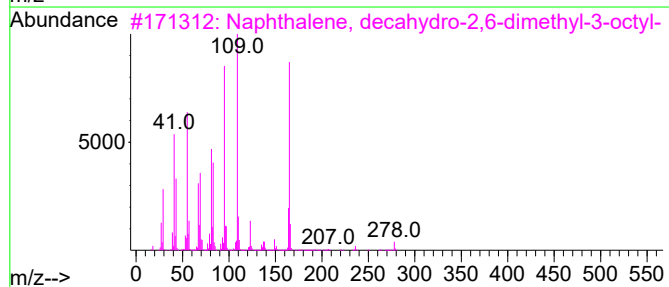
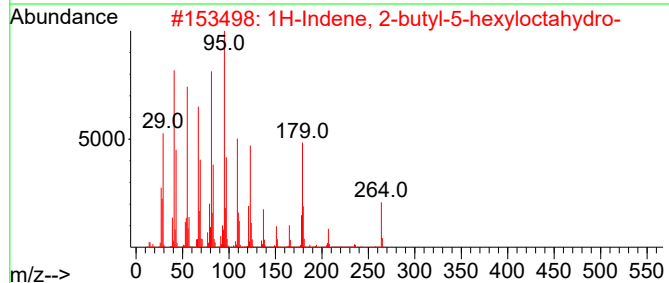
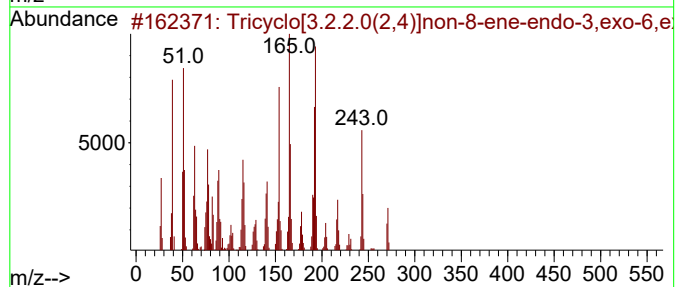
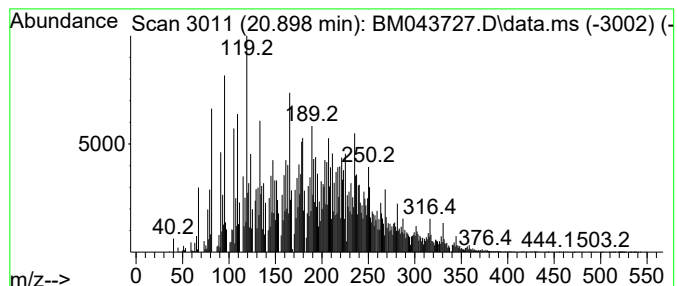
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 24 unknown-03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.898	20.00 ng/ul	24489000	Chrysene-d12	21.609	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[3.2.2.0(2,4)]non-8-ene-...	271	C18H13N3	1000154-27-8	56
2	1H-Indene, 2-butyl-5-hexyloctahy...	264	C19H36	055044-33-2	44
3	Naphthalene, decahydro-2,6-dimet...	278	C20H38	054964-85-1	38
4	2,4,4-Trimethyl-3-(3-oxobutyl)cy...	208	C13H20O2	072008-46-9	25
5	Butyric acid, 2-methyl-4-(2,5-xy...	206	C13H18O2	030316-14-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
 Data File : BM043727.D
 Acq On : 03 Jan 2024 11:31
 Operator : MA/JU
 Sample : 05919-14RE
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 GCF46RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid	4.081	11.2	ng/ul	1183950	1	7.963	2112870	20.0
unknown-01	5.040	2.5	ng/ul	262156	1	7.963	2112870	20.0
Pentanoic acid	5.457	3.9	ng/ul	414403	1	7.963	2112870	20.0
trans-1-Butene,...	5.675	30.5	ng/ul	3223800	1	7.963	2112870	20.0
3-Heptanone, 6-...	5.752	3.0	ng/ul	319903	1	7.963	2112870	20.0
Cyclohexanone	6.022	2.7	ng/ul	281463	1	7.963	2112870	20.0
cis-1-Butene,1-...	6.246	15.5	ng/ul	1634160	1	7.963	2112870	20.0
2,2-Dimethyl-1,...	6.475	4.5	ng/ul	471482	1	7.963	2112870	20.0
Hexanal, 2-ethyl-	6.863	3.5	ng/ul	364054	1	7.963	2112870	20.0
Butanoic acid, ...	7.016	4.6	ng/ul	485006	1	7.963	2112870	20.0
2-Hexenal, 2-et...	7.598	7.5	ng/ul	789877	1	7.963	2112870	20.0
unknown-02	7.722	3.3	ng/ul	347077	1	7.963	2112870	20.0
1-Hexanol, 2-et...	8.040	295.4	ng/ul	31209000	1	7.963	2112870	20.0
Heptanoic acid	8.581	2.9	ng/ul	302042	1	7.963	2112870	20.0
1,2-Cyclohexane...	8.763	3.4	ng/ul	362647	1	7.963	2112870	20.0
Hexanoic acid, ...	9.292	8.0	ng/ul	843310	1	7.963	2112870	20.0
1,3-Pentanediol...	10.292	2.5	ng/ul	2730790	2	10.775	22313000	20.0
1,3-Hexanediol,...	11.004	4.2	ng/ul	4694650	2	10.775	22313000	20.0
1,3-Hexanediol,...	11.098	5.3	ng/ul	5953980	2	10.775	22313000	20.0
3-Heptanone, 5-...	11.375	9.5	ng/ul	10609800	2	10.775	22313000	20.0
(DEL) Alkane: S...	12.181	6.7	ng/ul	7447400	2	10.775	22313000	20.0
(DEL) Alkane: S...	14.516	20.0	ng/ul	159150000	3	14.616	159150000	20.0
Tricyclo[3.2.2....	20.386	6.3	ng/ul	7678320	5	21.609	24489000	20.0
unknown-03	20.898	20.0	ng/ul	24489000	5	21.609	24489000	20.0