

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
 Data File : BM047801.D
 Acq On : 03 Oct 2024 07:44
 Operator : RC/JU
 Sample : P4020-15
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DDCL3

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.1 % of largest Peak

Max Peaks: 100

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-BM092724.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM047801.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	41	45	51	rBV	28793	40568	0.89%	0.074%
2	3.528	89	92	99	rVB2	23493	36681	0.81%	0.067%
3	3.669	113	116	131	rBV	286530	433394	9.55%	0.795%
4	3.881	145	152	157	rVB	91003	148782	3.28%	0.273%
5	3.999	168	172	176	rVB2	20046	29311	0.65%	0.054%
6	4.263	213	217	221	rVB3	10932	17894	0.39%	0.033%
7	4.322	223	227	233	rVV	19721	27949	0.62%	0.051%
8	4.922	324	329	339	rVB	335459	477298	10.52%	0.876%
9	5.698	451	461	465	rVB7	14235	34734	0.77%	0.064%
10	5.851	482	487	492	rBV3	18270	32296	0.71%	0.059%
11	6.128	528	534	542	rBV	913101	1380655	30.42%	2.534%
12	6.310	560	565	570	rVB7	9927	17533	0.39%	0.032%
13	6.563	603	608	612	rVV2	24354	35613	0.78%	0.065%
14	6.792	643	647	652	rBV4	15617	29553	0.65%	0.054%
15	6.969	670	677	689	rBV	439463	717220	15.80%	1.316%
16	7.134	699	705	710	rBV	390689	593304	13.07%	1.089%
17	7.340	732	740	750	rBV	479092	775728	17.09%	1.424%
18	7.563	772	778	784	rVB4	32828	66356	1.46%	0.122%
19	7.734	800	807	812	rBV	83498	138362	3.05%	0.254%
20	7.804	812	819	826	rVV	946719	1494736	32.94%	2.744%
21	7.875	826	831	838	rVB	44506	72973	1.61%	0.134%
22	8.039	845	859	867	rVB3	358024	739953	16.30%	1.358%
23	8.145	872	877	883	rBV7	11876	26361	0.58%	0.048%
24	8.234	886	892	897	rBV	68579	112907	2.49%	0.207%
25	8.275	897	899	906	rVB5	14839	21167	0.47%	0.039%
26	8.410	918	922	926	rVV5	20747	37039	0.82%	0.068%
27	8.510	932	939	950	rBV	567647	948302	20.90%	1.741%
28	8.610	952	956	962	rVB2	24990	43743	0.96%	0.080%
29	8.686	965	969	979	rVB	32498	57647	1.27%	0.106%
30	8.957	1005	1015	1026	rBV	454218	848584	18.70%	1.558%
31	9.134	1027	1045	1055	rBV	639889	1602839	35.32%	2.942%
32	9.234	1058	1062	1065	rBV4	17720	22324	0.49%	0.041%
33	9.392	1085	1089	1093	rVV5	13509	22654	0.50%	0.042%
34	9.469	1099	1102	1107	rVV4	11634	21393	0.47%	0.039%
35	9.522	1107	1111	1121	rVB2	45504	94442	2.08%	0.173%
36	9.681	1130	1138	1145	rBV2	384459	743534	16.38%	1.365%

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
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37	9.757	1145	1151	1155	rVV	88991	139369	3.07%	0.256%
38	9.798	1155	1158	1161	rVV2	16922	23357	0.51%	0.043%
39	9.839	1161	1165	1171	rVB3	21628	37076	0.82%	0.068%
40	9.904	1171	1176	1181	rBV8	16972	28456	0.63%	0.052%

41	10.098	1202	1209	1220	rVV	177987	312375	6.88%	0.573%
42	10.216	1220	1229	1238	rBV	596939	1033965	22.78%	1.898%
43	10.369	1245	1255	1262	rVB6	22038	56053	1.24%	0.103%
44	10.475	1265	1273	1280	rBV2	177324	329412	7.26%	0.605%
45	10.598	1286	1294	1301	rVB	1289233	2135133	47.05%	3.919%

46	10.728	1310	1316	1323	rVV	532222	916141	20.19%	1.682%
47	10.798	1323	1328	1334	rVV	55663	119112	2.62%	0.219%
48	10.857	1334	1338	1339	rVV4	18279	31099	0.69%	0.057%
49	10.892	1339	1344	1355	rVV	93163	182670	4.03%	0.335%
50	10.980	1355	1359	1368	rVV6	15566	38310	0.84%	0.070%

51	11.492	1441	1446	1453	rBV2	27624	48138	1.06%	0.088%
52	11.739	1485	1488	1495	rVB9	12087	19655	0.43%	0.036%
53	11.875	1505	1511	1514	rBV6	7195	15365	0.34%	0.028%
54	12.139	1546	1556	1560	rVV8	23554	65596	1.45%	0.120%
55	12.186	1560	1564	1572	rVB6	16366	27637	0.61%	0.051%

56	12.339	1583	1590	1598	rVB9	15958	43967	0.97%	0.081%
57	12.533	1619	1623	1629	rBV6	14522	28087	0.62%	0.052%
58	12.692	1644	1650	1653	rBV4	16116	27999	0.62%	0.051%
59	12.733	1653	1657	1665	rVV2	29228	51324	1.13%	0.094%
60	12.816	1665	1671	1674	rVV7	11273	22648	0.50%	0.042%

61	12.863	1674	1679	1685	rVB	38508	64192	1.41%	0.118%
62	13.192	1730	1735	1743	rVB	76044	109480	2.41%	0.201%
63	13.292	1743	1752	1757	rBV6	20761	41094	0.91%	0.075%
64	13.404	1757	1771	1774	rVV3	56903	110876	2.44%	0.204%
65	13.433	1774	1776	1784	rVV7	15909	33577	0.74%	0.062%

66	13.704	1816	1822	1831	rVB	106747	167455	3.69%	0.307%
67	13.845	1840	1846	1856	rVB	1158027	1556860	34.31%	2.858%
68	13.945	1858	1863	1868	rBV3	18236	29289	0.65%	0.054%
69	14.133	1884	1895	1902	rBV	1282133	1941615	42.78%	3.564%
70	14.204	1902	1907	1912	rVV4	30035	62394	1.37%	0.115%

71	14.439	1940	1947	1956	rBV	1952163	2847237	62.74%	5.226%
72	14.627	1974	1979	1992	rBV	386656	609008	13.42%	1.118%
73	14.745	1992	1999	2004	rBV4	48664	94054	2.07%	0.173%
74	14.980	2035	2039	2043	rBV4	20391	28998	0.64%	0.053%
75	15.063	2048	2053	2059	rVV	139599	210975	4.65%	0.387%

76	15.239	2077	2083	2089	rBV6	11220	25135	0.55%	0.046%
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 Title : SVOA CALIBRATION

77	15.427	2109	2115	2124	rBV	1706063	2402456	52.94%	4.410%
78	15.539	2128	2134	2145	rVV2	360120	571311	12.59%	1.049%
79	15.668	2152	2156	2162	rBV8	10327	15555	0.34%	0.029%
80	15.792	2172	2177	2184	rVV	359292	492008	10.84%	0.903%
81	16.245	2249	2254	2262	rVV	51675	83333	1.84%	0.153%
82	16.580	2307	2311	2316	rBV6	15390	21000	0.46%	0.039%
83	16.827	2344	2353	2363	rBV	1617610	2352343	51.83%	4.318%
84	17.174	2404	2412	2422	rBV	2374098	3423641	75.44%	6.284%
85	17.274	2422	2429	2438	rVV	1914585	2658927	58.59%	4.880%
86	17.345	2438	2441	2447	rVB8	14493	18863	0.42%	0.035%
87	17.468	2457	2462	2468	rBV5	8845	18553	0.41%	0.034%
88	17.557	2473	2477	2483	rVB9	10787	16889	0.37%	0.031%
89	17.792	2512	2517	2523	rBV	154475	213516	4.70%	0.392%
90	18.074	2559	2565	2574	rBV	449218	723519	15.94%	1.328%
91	19.127	2740	2744	2749	rBV5	30357	47386	1.04%	0.087%
92	19.198	2753	2756	2759	rBV2	34937	49326	1.09%	0.091%
93	19.345	2777	2781	2789	rBV3	95969	145542	3.21%	0.267%
94	19.498	2804	2807	2810	rVB3	23093	21668	0.48%	0.040%
95	19.562	2812	2818	2824	rBV	2391684	3242653	71.45%	5.952%
96	20.556	2984	2987	2991	rBV2	74917	83677	1.84%	0.154%
97	21.074	3071	3075	3082	rBV	357610	527405	11.62%	0.968%
98	21.397	3125	3130	3136	rBV	2545369	3896237	85.85%	7.152%
99	24.197	3598	3606	3618	rVB	1328213	3307745	72.89%	6.071%
100	24.403	3632	3641	3660	rVB	1728297	4538225	100.00%	8.330%

Sum of corrected areas: 54480790

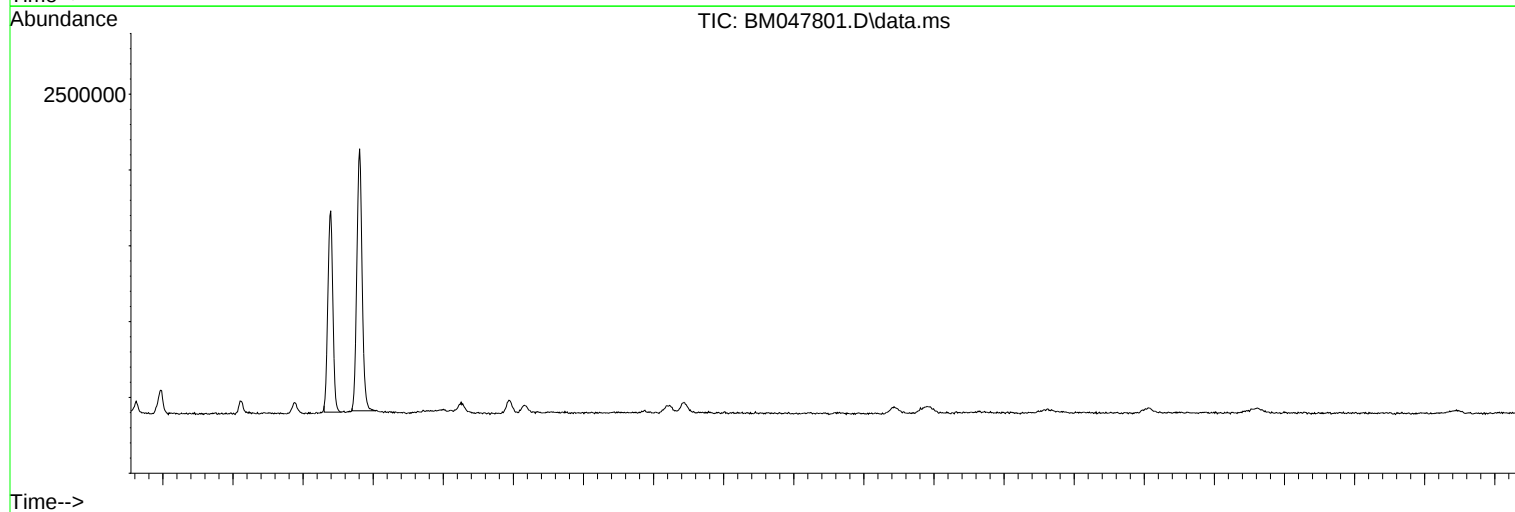
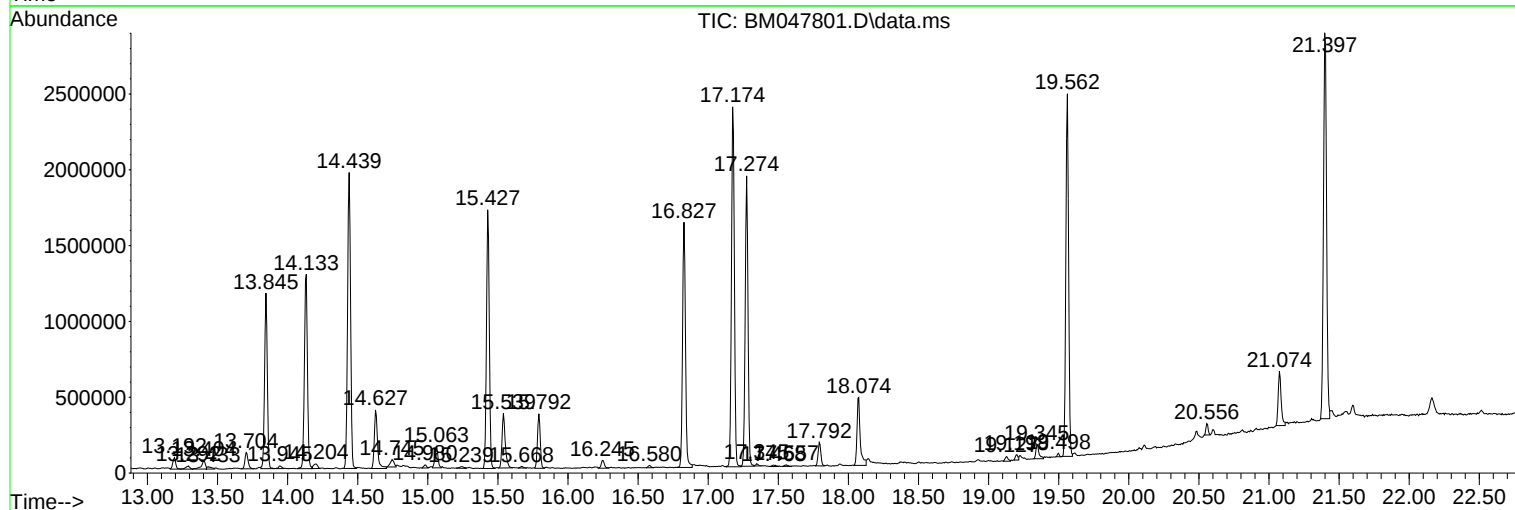
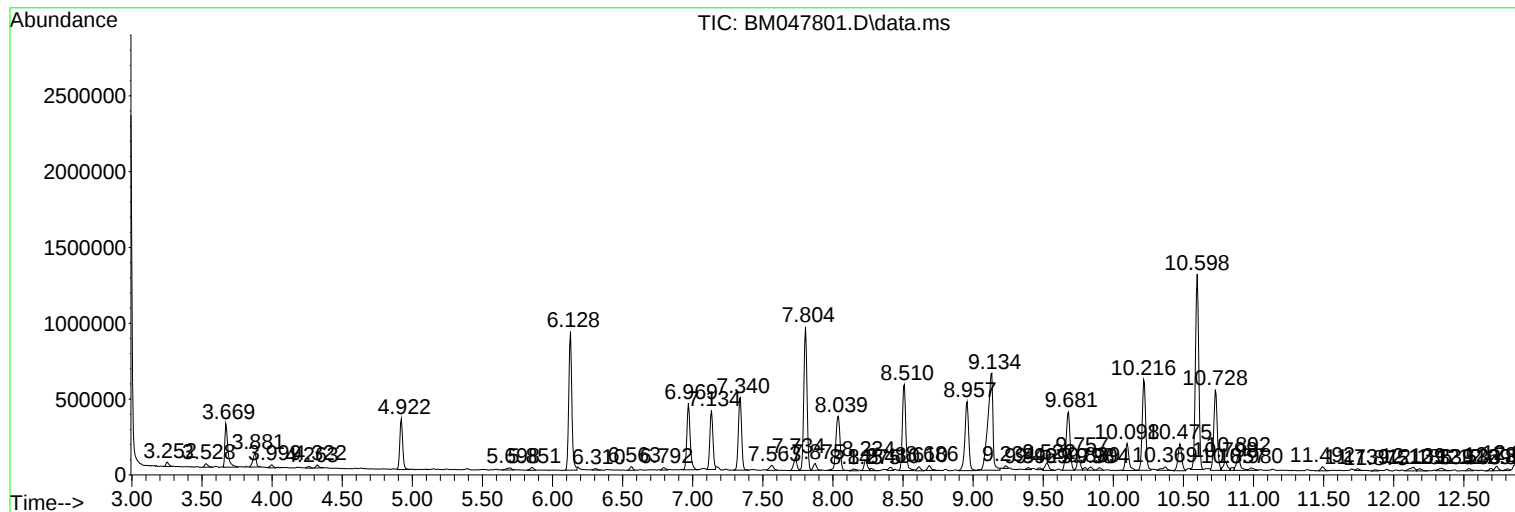
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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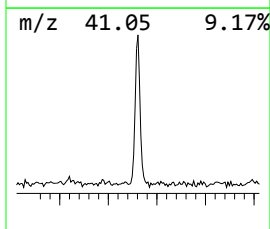
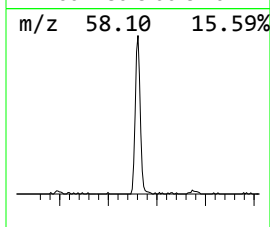
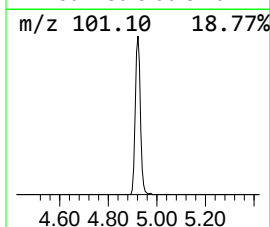
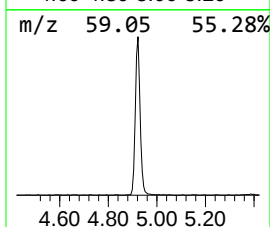
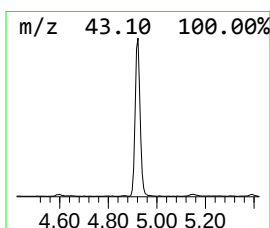
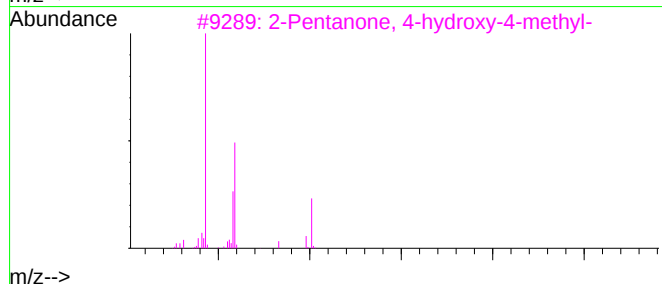
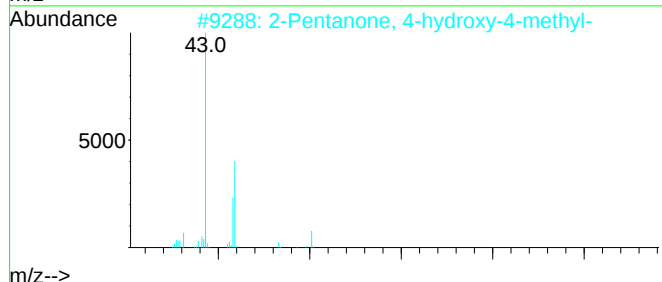
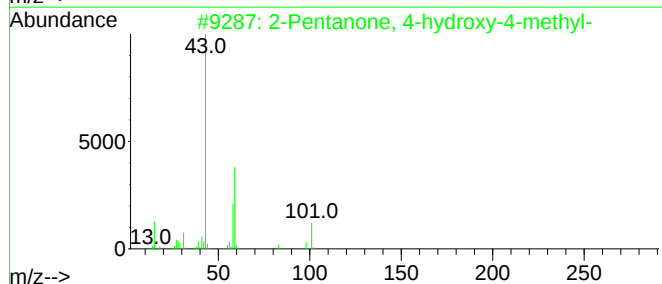
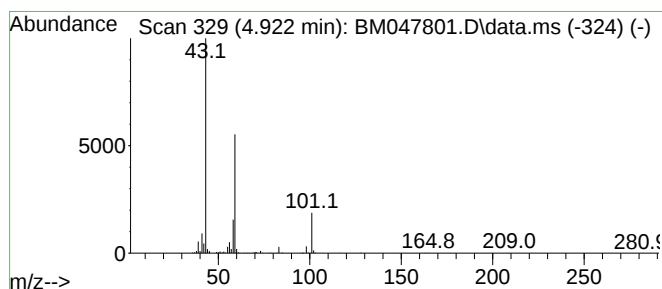
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.922	6.39 ng/ul	477298	1,4-Dichlorobenzene-d4	7.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32



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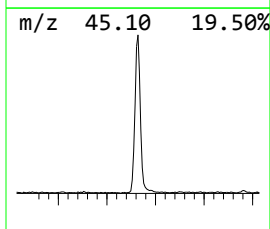
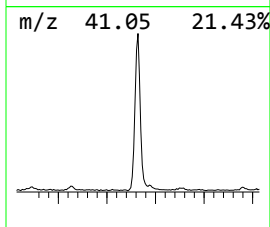
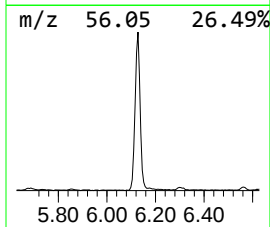
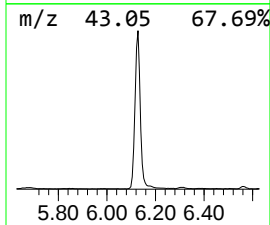
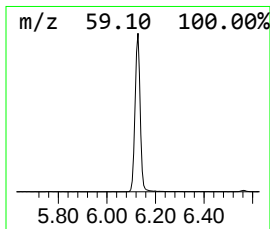
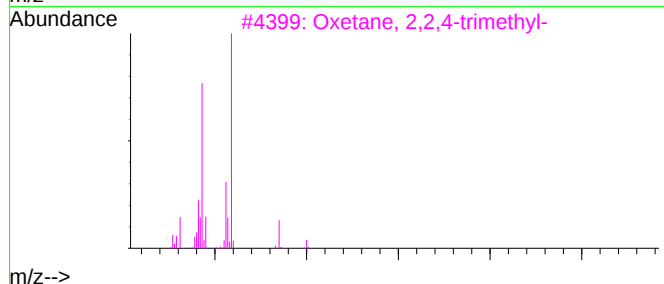
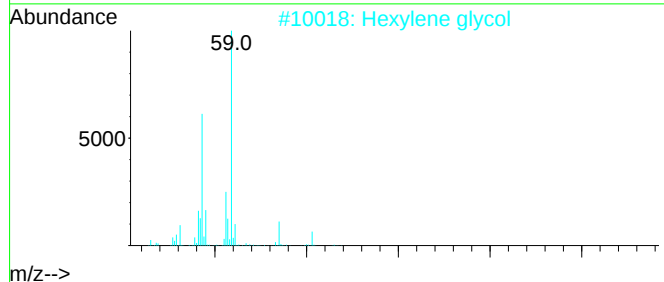
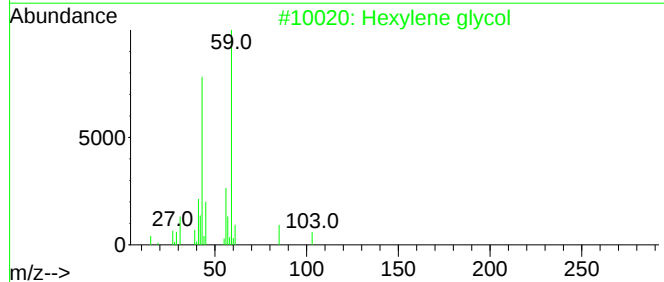
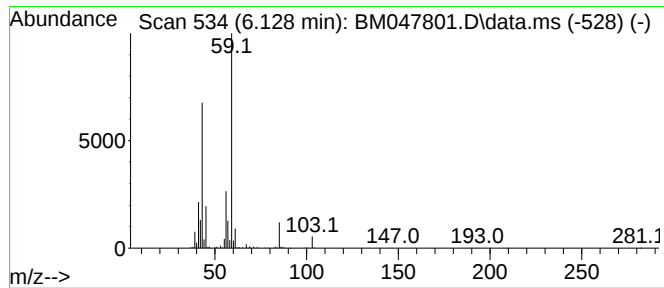
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexylene glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.128	18.47 ng/ul	1380660	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	90
2	Hexylene glycol	118	C6H14O2	000107-41-5	90
3	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	72
4	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	59
5	Hexylene glycol	118	C6H14O2	000107-41-5	50



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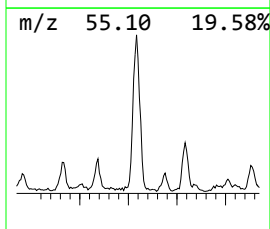
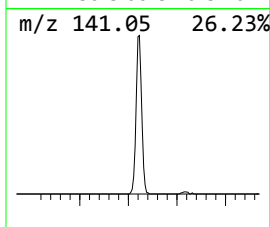
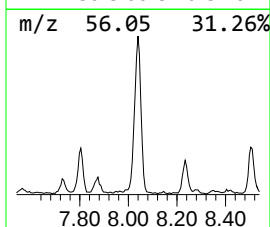
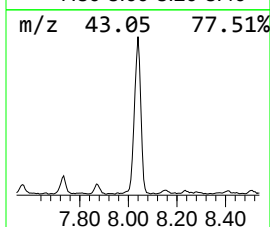
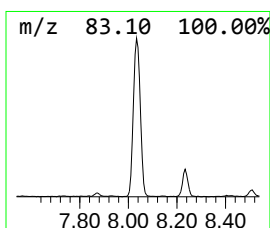
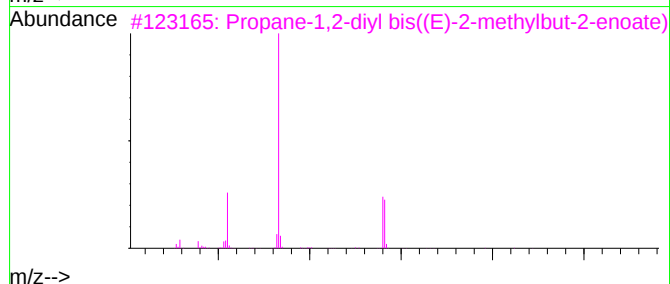
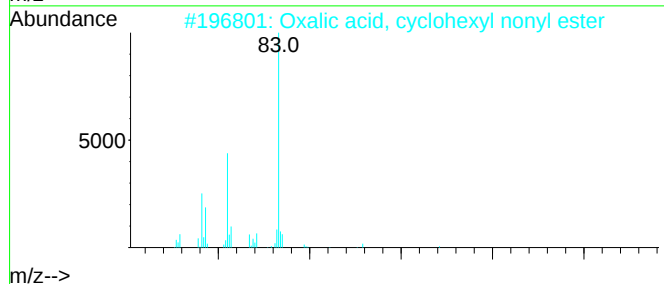
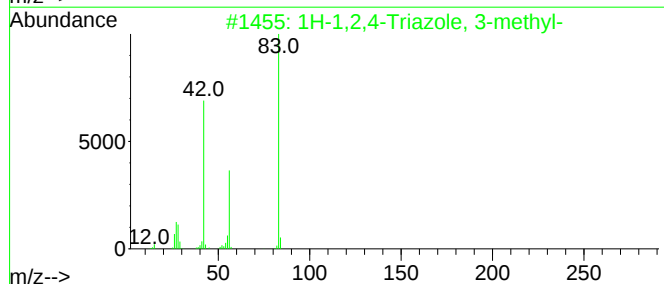
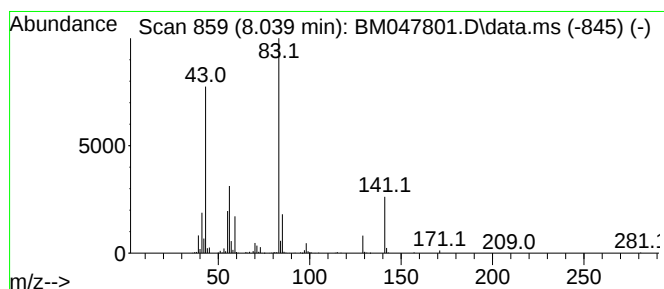
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.039	9.90 ng/ul	739953	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	38
2	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	37
3	Propane-1,2-diyl bis((E)-2-methy...	240	C13H20O4	1000373-72-4	28
4	3-(Butylamino)propionitrile	126	C7H14N2	000693-51-6	28
5	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
Data File : BM047801.D
Acq On : 03 Oct 2024 07:44
Operator : RC/JU
Sample : P4020-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCL3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
Quant Title : SVOA CALIBRATION

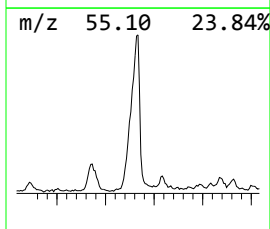
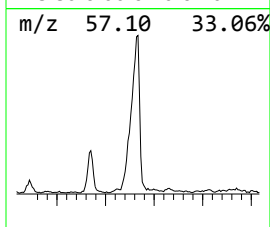
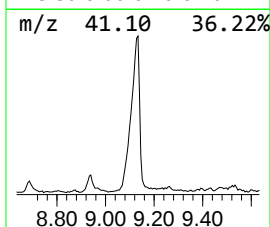
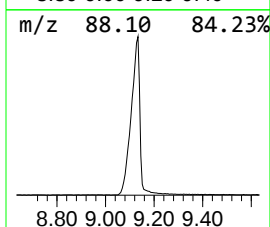
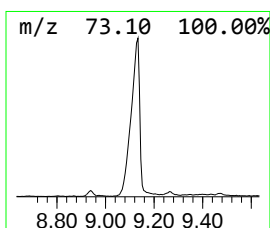
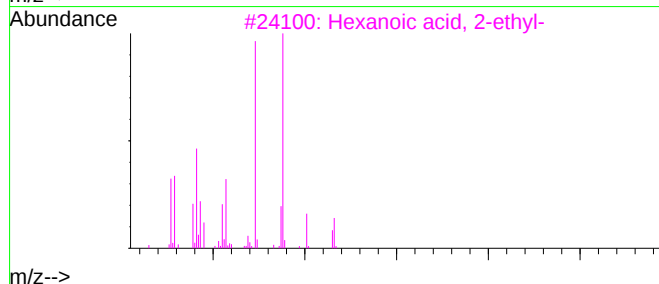
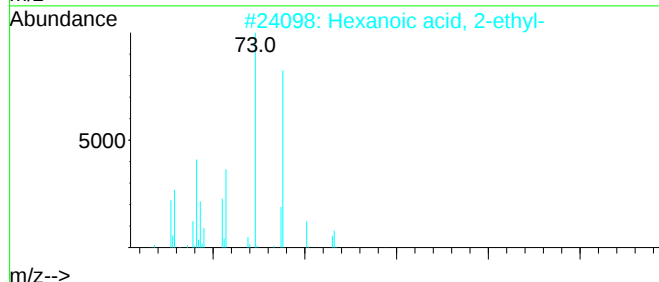
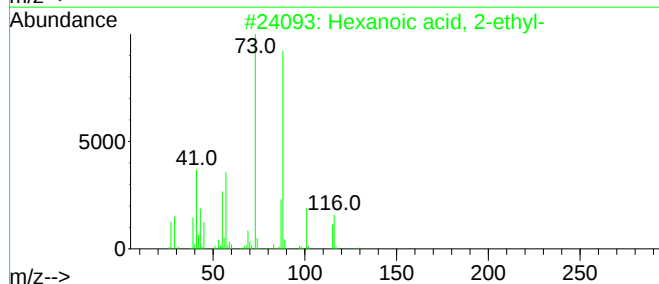
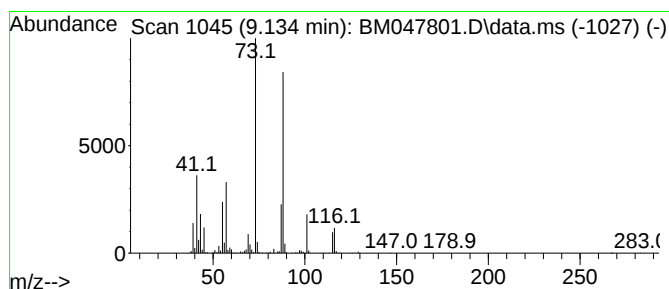
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.134	21.45 ng/ul	1602840	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
Data File : BM047801.D
Acq On : 03 Oct 2024 07:44
Operator : RC/JU
Sample : P4020-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DDCL3

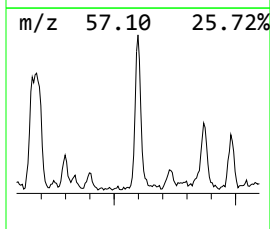
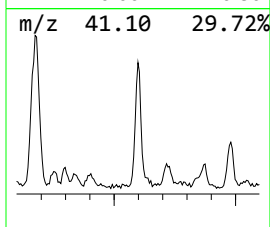
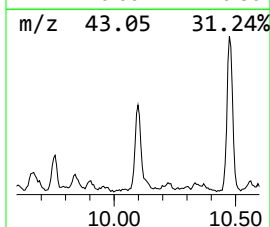
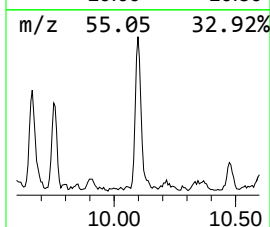
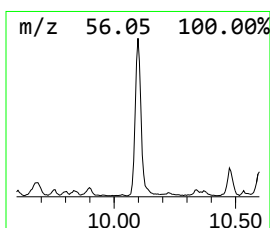
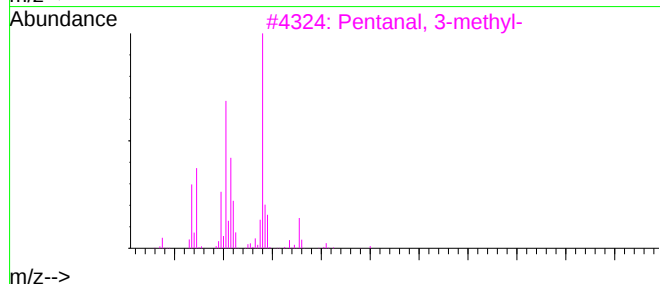
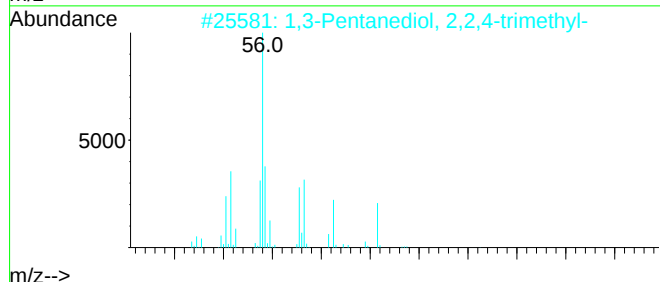
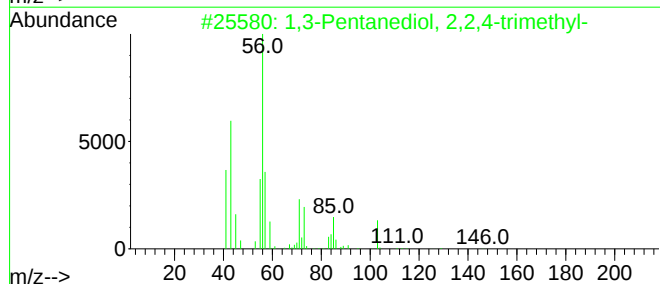
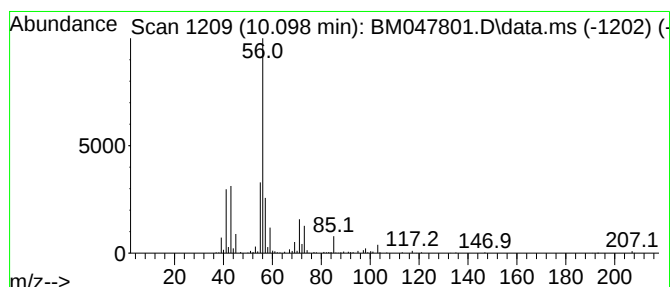
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1,3-Pentanediol, 2,2,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.098	2.93 ng/ul	312375	Naphthalene-d8	10.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	78
2	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	74
3	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	53
4	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	47
5	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
Data File : BM047801.D
Acq On : 03 Oct 2024 07:44
Operator : RC/JU
Sample : P4020-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.MA.M
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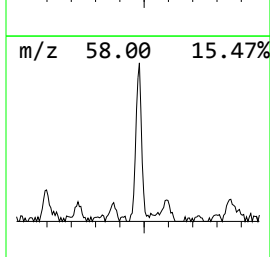
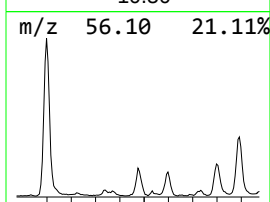
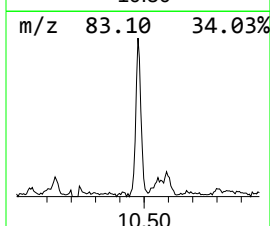
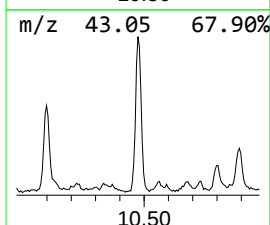
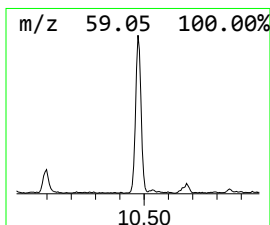
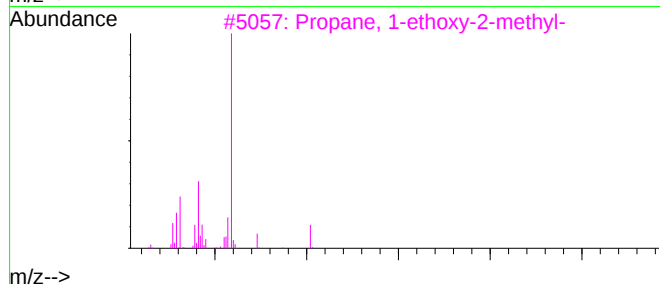
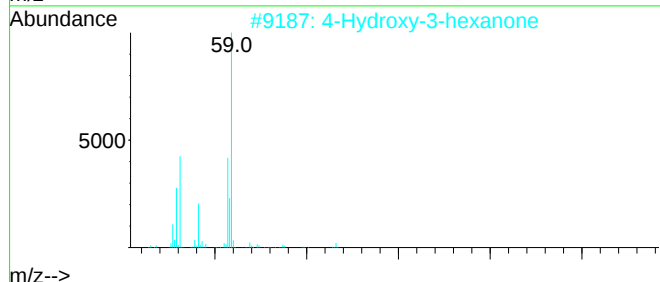
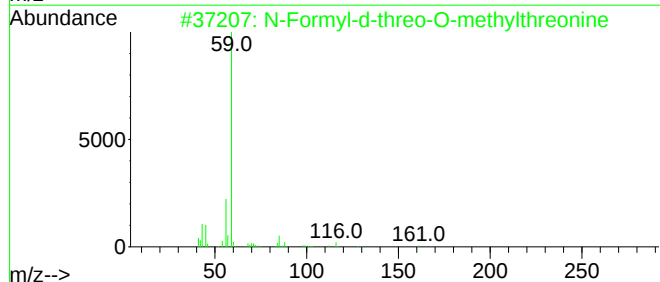
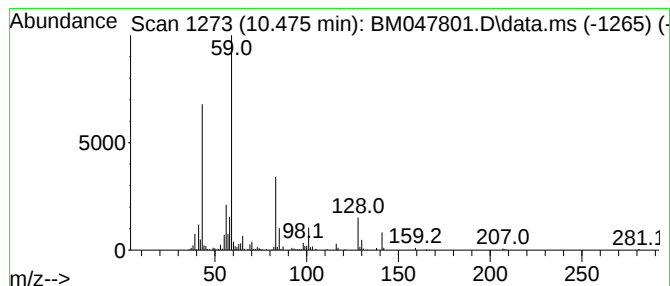
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.09 ng/ul	329412	Naphthalene-d8	10.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Formyl-d-threo-O-methylthreonine	161	C6H11N04	1000214-69-5	40
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	38
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	38
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
Data File : BM047801.D
Acq On : 03 Oct 2024 07:44
Operator : RC/JU
Sample : P4020-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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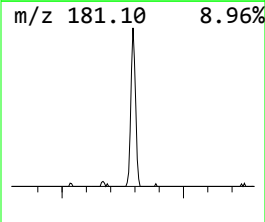
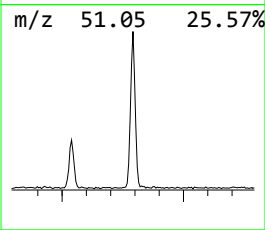
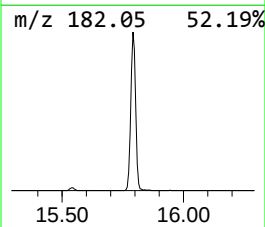
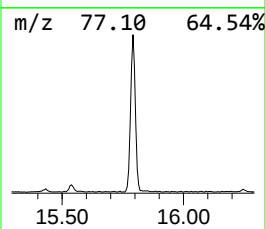
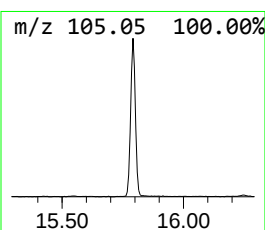
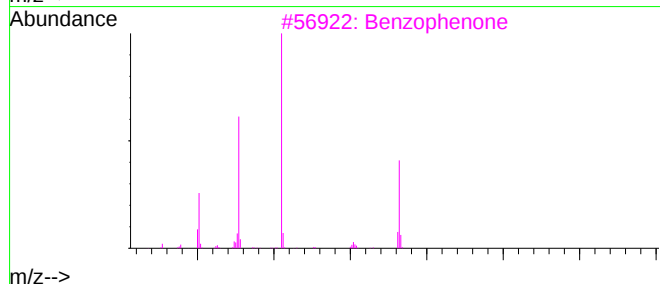
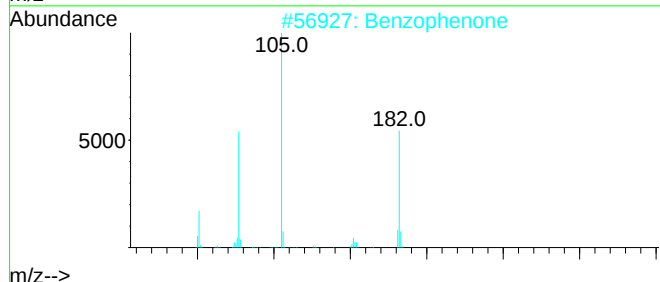
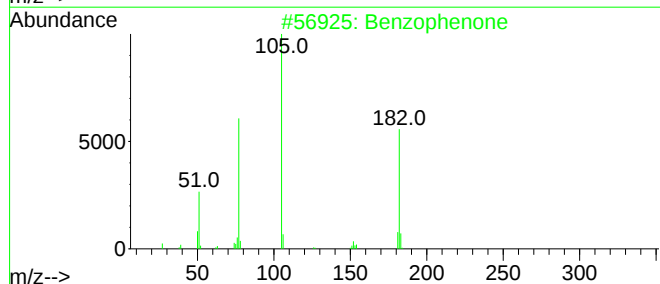
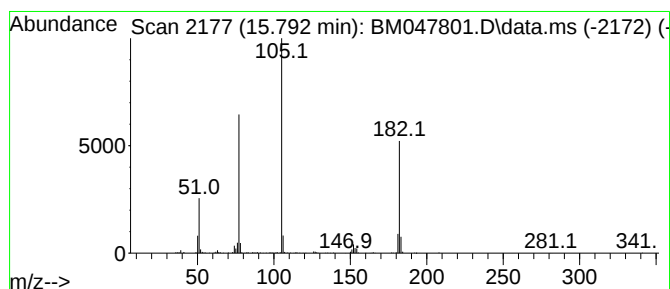
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	3.46 ng/ul	492008	Acenaphthene-d10	14.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	93
5	Benzophenone	182	C13H10O	000119-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
Data File : BM047801.D
Acq On : 03 Oct 2024 07:44
Operator : RC/JU
Sample : P4020-15
Misc :
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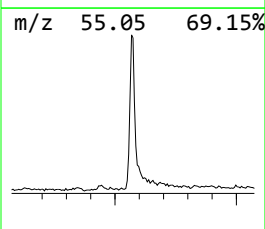
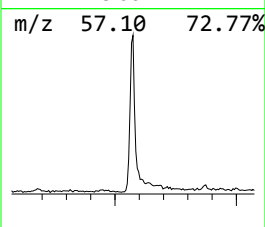
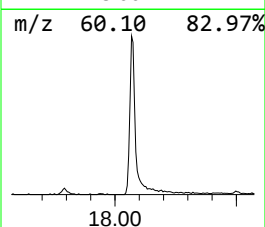
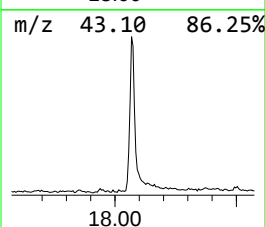
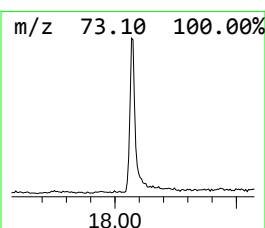
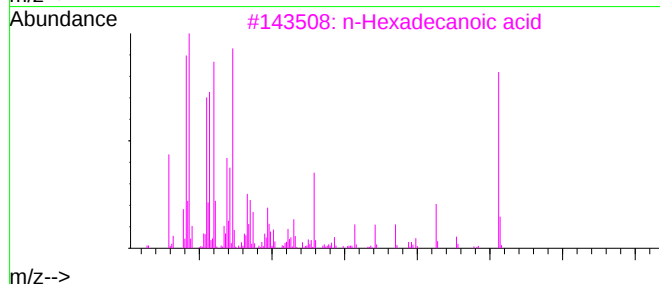
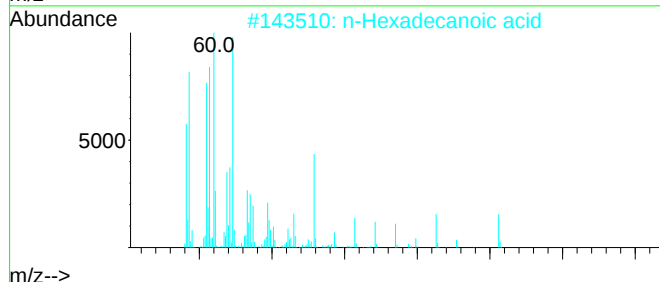
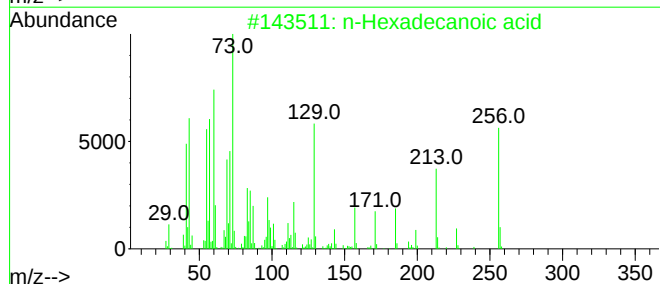
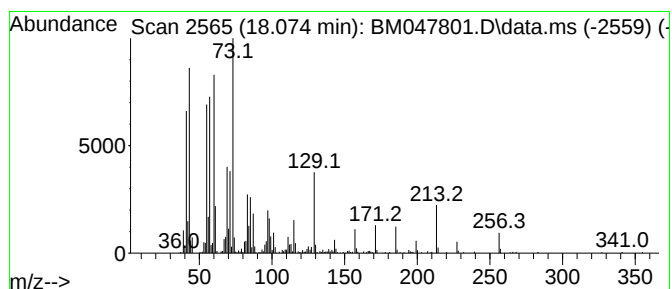
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.074	4.23 ng/ul	723519	Phenanthrene-d10		17.174	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
4	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
5	Tridecanoic acid		214	C13H26O2	000638-53-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
Data File : BM047801.D
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ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId :
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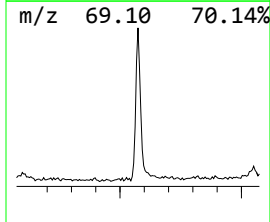
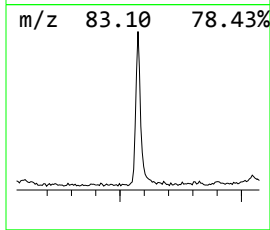
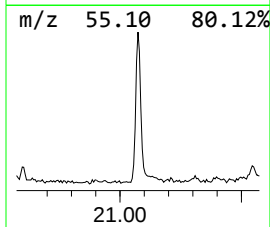
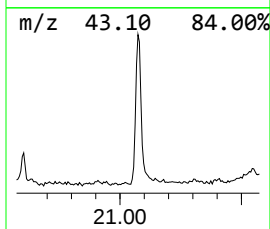
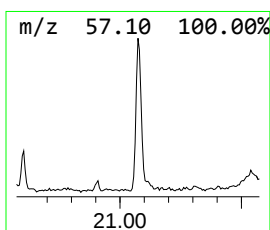
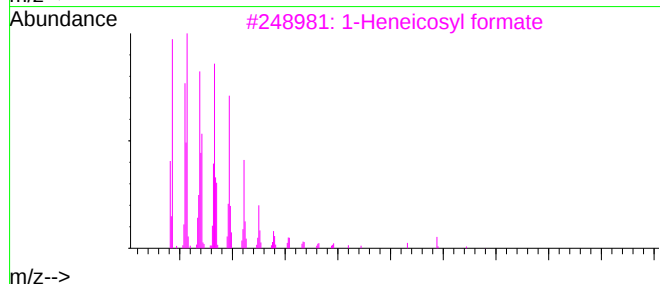
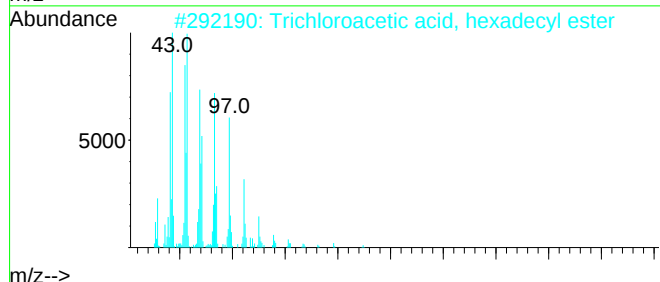
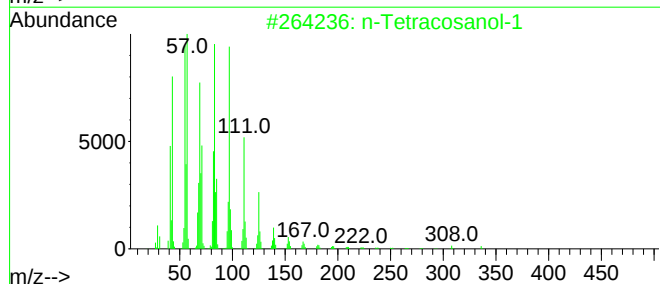
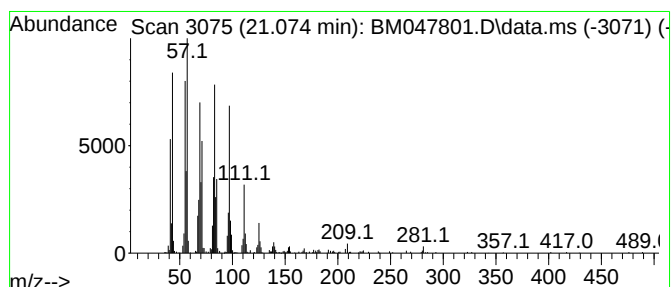
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	2.71 ng/ul	527405	Chrysene-d12	21.397

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100224\
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Operator : RC/JU
Sample : P4020-15
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM092724.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
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Hexylene glycol	6.128	18.5	ng/u1	1380660	1	7.804	1494740	20.0
unknown-01	8.039	9.9	ng/u1	739953	1	7.804	1494740	20.0
Hexanoic acid, ...	9.134	21.4	ng/u1	1602840	1	7.804	1494740	20.0
1,3-Pentanediol...	10.098	2.9	ng/u1	312375	2	10.598	2135130	20.0
unknown-02	10.475	3.1	ng/u1	329412	2	10.598	2135130	20.0
Benzophenone	15.792	3.5	ng/u1	492008	3	14.439	2847240	20.0
n-Hexadecanoic ...	18.074	4.2	ng/u1	723519	4	17.174	3423640	20.0
n-Tetracosanol-1	21.074	2.7	ng/u1	527405	5	21.397	3896240	20.0