

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
 Acq On : 05 Oct 2023 14:14
 Operator : MA/JU
 Sample : 04679-09
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PMW-3(2030927)

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_P\Methods\SFAM-EPA-BP100423.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP017564.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.287	31	34	37	rVV	20380	23592	0.52%	0.059%
2	3.323	37	40	46	rVB	20407	26581	0.58%	0.067%
3	3.728	105	109	125	rBV	140314	224362	4.93%	0.564%
4	4.028	156	160	164	rVB	9956	12107	0.27%	0.030%
5	5.193	352	358	368	rVB	47663	72254	1.59%	0.182%
6	5.622	427	431	438	rVB9	9193	17260	0.38%	0.043%
7	6.364	553	557	563	rVB7	7818	11333	0.25%	0.028%
8	7.099	676	682	692	rBV	135711	229386	5.04%	0.577%
9	7.281	703	713	721	rBV	468860	720182	15.82%	1.811%
10	7.458	736	743	751	rBV	467638	728384	16.00%	1.832%
11	7.546	755	758	764	rVB5	10120	18403	0.40%	0.046%
12	7.940	816	825	834	rBV	367733	625578	13.74%	1.573%
13	8.022	834	839	848	rVB6	18932	39840	0.88%	0.100%
14	8.152	855	861	865	rBV	14768	23686	0.52%	0.060%
15	8.293	880	885	892	rVV	29527	45148	0.99%	0.114%
16	8.393	896	902	909	rVB4	10986	18039	0.40%	0.045%
17	8.552	924	929	933	rBV5	9496	14848	0.33%	0.037%
18	8.658	939	947	955	rBV	413810	700724	15.39%	1.762%
19	9.058	1003	1015	1020	rBV2	37005	84719	1.86%	0.213%
20	9.146	1020	1030	1039	rBV	549028	900351	19.78%	2.264%
21	9.258	1044	1049	1060	rVB	77909	148461	3.26%	0.373%
22	9.340	1060	1063	1066	rBV4	6594	11828	0.26%	0.030%
23	9.616	1102	1110	1120	rVB7	12274	31061	0.68%	0.078%
24	9.716	1123	1127	1132	rVB2	8170	13750	0.30%	0.035%
25	9.863	1146	1152	1159	rBV	458790	760023	16.70%	1.911%
26	9.958	1164	1168	1172	rBV5	12234	19232	0.42%	0.048%
27	10.063	1180	1186	1187	rBV6	9463	14555	0.32%	0.037%
28	10.134	1194	1198	1204	rVB	24339	36021	0.79%	0.091%
29	10.210	1206	1211	1216	rVV6	10960	16949	0.37%	0.043%
30	10.340	1225	1233	1235	rBV9	8642	19165	0.42%	0.048%
31	10.393	1235	1242	1255	rVV	680471	1146408	25.18%	2.883%
32	10.493	1255	1259	1265	rVB7	16099	26135	0.57%	0.066%
33	10.775	1300	1307	1314	rBV	533831	871436	19.14%	2.191%
34	10.852	1314	1320	1325	rVB3	22955	48549	1.07%	0.122%
35	10.946	1328	1336	1345	rBV	598542	1069212	23.49%	2.689%
36	11.216	1378	1382	1389	rVB3	13925	26860	0.59%	0.068%

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37	11.328	1394	1401	1411	rVV2	99719	221208	4.86%	0.556%
38	11.410	1411	1415	1419	rVV5	11731	26432	0.58%	0.066%
39	11.452	1419	1422	1427	rVV7	16723	30232	0.66%	0.076%
40	11.516	1427	1433	1436	rVV3	12329	26695	0.59%	0.067%
41	11.546	1436	1438	1450	rVB3	7940	18559	0.41%	0.047%
42	11.669	1453	1459	1464	rVB5	13214	23021	0.51%	0.058%
43	11.804	1476	1482	1488	rBV5	25768	56143	1.23%	0.141%
44	11.857	1488	1491	1494	rVV4	8444	13136	0.29%	0.033%
45	12.040	1518	1522	1527	rBV8	8389	16035	0.35%	0.040%
46	12.122	1531	1536	1543	rVV5	12386	23613	0.52%	0.059%
47	12.187	1543	1547	1558	rVB5	18912	48380	1.06%	0.122%
48	12.310	1563	1568	1571	rBV4	12878	21912	0.48%	0.055%
49	12.363	1571	1577	1583	rVB5	16328	32641	0.72%	0.082%
50	12.440	1586	1590	1594	rVB6	19705	31854	0.70%	0.080%
51	12.575	1609	1613	1617	rBV6	17935	32217	0.71%	0.081%
52	12.675	1620	1630	1634	rBV5	58377	138596	3.04%	0.349%
53	12.751	1640	1643	1647	rVB4	17658	23144	0.51%	0.058%
54	12.875	1659	1664	1670	rVB3	23978	41405	0.91%	0.104%
55	12.957	1670	1678	1686	rVB	156791	248142	5.45%	0.624%
56	13.051	1689	1694	1697	rBV	62904	98192	2.16%	0.247%
57	13.081	1697	1699	1704	rVB4	24589	28435	0.62%	0.072%
58	13.210	1715	1721	1723	rBV7	10371	19013	0.42%	0.048%
59	13.246	1723	1727	1729	rBV4	15758	21842	0.48%	0.055%
60	13.316	1735	1739	1744	rVB2	31100	47591	1.05%	0.120%
61	13.369	1744	1748	1755	rVB2	41585	64336	1.41%	0.162%
62	13.463	1755	1764	1770	rBV4	56129	106240	2.33%	0.267%
63	13.616	1783	1790	1791	rBV5	36530	61499	1.35%	0.155%
64	13.640	1791	1794	1798	rVB	33547	50487	1.11%	0.127%
65	13.757	1810	1814	1817	rBV5	15372	21607	0.47%	0.054%
66	13.904	1834	1839	1842	rBV3	30865	56425	1.24%	0.142%
67	14.046	1850	1863	1871	rBV	1502264	2018317	44.34%	5.075%
68	14.175	1881	1885	1894	rVB5	33925	55748	1.22%	0.140%
69	14.251	1894	1898	1900	rBV5	11187	13950	0.31%	0.035%
70	14.293	1900	1905	1907	rBV	240117	334256	7.34%	0.841%
71	14.328	1907	1911	1917	rVB	1456190	2074258	45.57%	5.216%
72	14.422	1923	1927	1934	rVB2	16145	23855	0.52%	0.060%
73	14.634	1956	1963	1970	rVB	809980	1200704	26.38%	3.019%
74	14.698	1971	1974	1979	rBV6	10408	17815	0.39%	0.045%
75	14.887	2001	2006	2015	rBV	90378	177836	3.91%	0.447%
76	15.016	2025	2028	2035	rVB5	14207	31233	0.69%	0.079%

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77	15.210	2058	2061	2065	rBV3	20394	29594	0.65%	0.074%
78	15.375	2085	2089	2092	rBV	37962	49653	1.09%	0.125%
79	15.545	2114	2118	2119	rBV5	11644	15832	0.35%	0.040%
80	15.634	2127	2133	2141	rBV	2064824	2873080	63.12%	7.225%
81	15.775	2152	2157	2171	rVB	704504	960751	21.11%	2.416%
82	15.987	2186	2193	2204	rVB2	91055	165981	3.65%	0.417%
83	16.216	2229	2232	2240	rVB9	19798	39555	0.87%	0.099%
84	16.563	2288	2291	2300	rVB6	25800	49004	1.08%	0.123%
85	16.704	2310	2315	2320	rBV2	104417	146297	3.21%	0.368%
86	16.775	2322	2327	2335	rVB5	43910	78591	1.73%	0.198%
87	17.081	2377	2379	2384	rVB5	15131	20162	0.44%	0.051%
88	17.422	2431	2437	2447	rVB	1041265	1536417	33.75%	3.864%
89	17.522	2448	2454	2464	rBV	2474304	3455928	75.92%	8.691%
90	18.145	2558	2560	2564	rVB5	13335	13415	0.29%	0.034%
91	18.269	2576	2581	2593	rBV	369506	538999	11.84%	1.355%
92	19.339	2760	2763	2766	rBV3	32587	37355	0.82%	0.094%
93	19.398	2770	2773	2784	rVB3	62618	134292	2.95%	0.338%
94	19.510	2789	2792	2803	rVV	129175	184827	4.06%	0.465%
95	19.775	2831	2837	2843	rBV	3408596	4342625	95.40%	10.920%
96	21.210	3078	3081	3088	rBV3	126656	171943	3.78%	0.432%
97	21.557	3135	3140	3148	rVB	1387535	1770132	38.89%	4.451%
98	22.810	3349	3353	3362	rVB	234616	334366	7.35%	0.841%
99	23.963	3541	3549	3562	rVB2	2189354	4551957	100.00%	11.447%
100	24.133	3572	3578	3590	rVB	919645	1872500	41.14%	4.709%

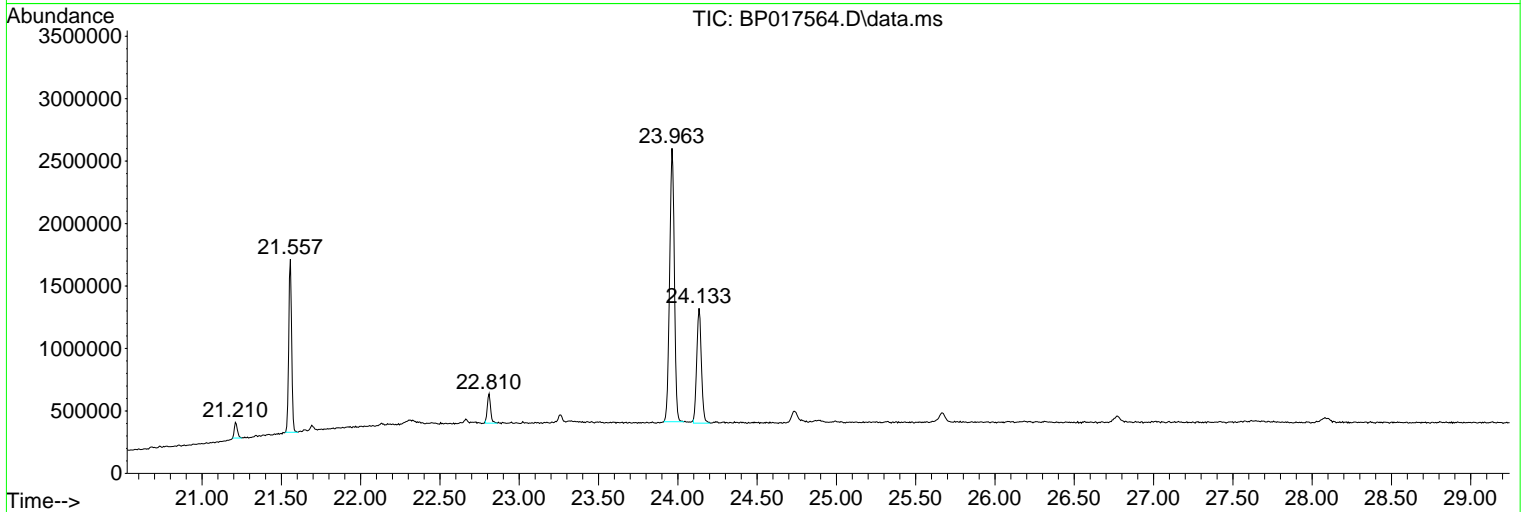
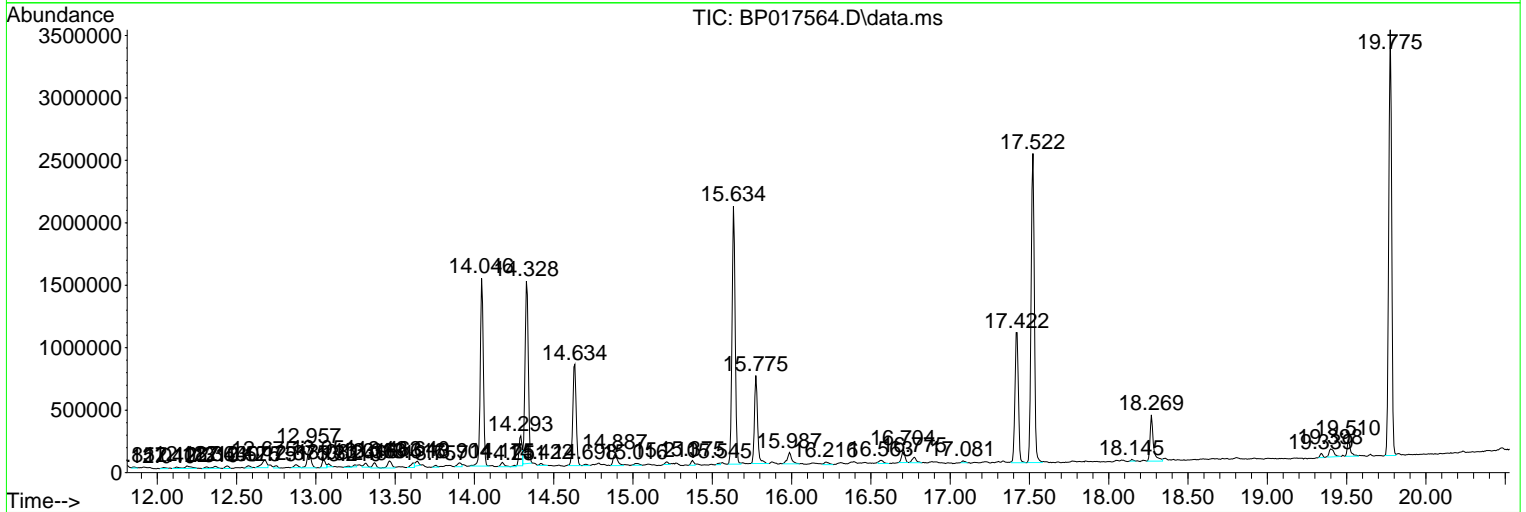
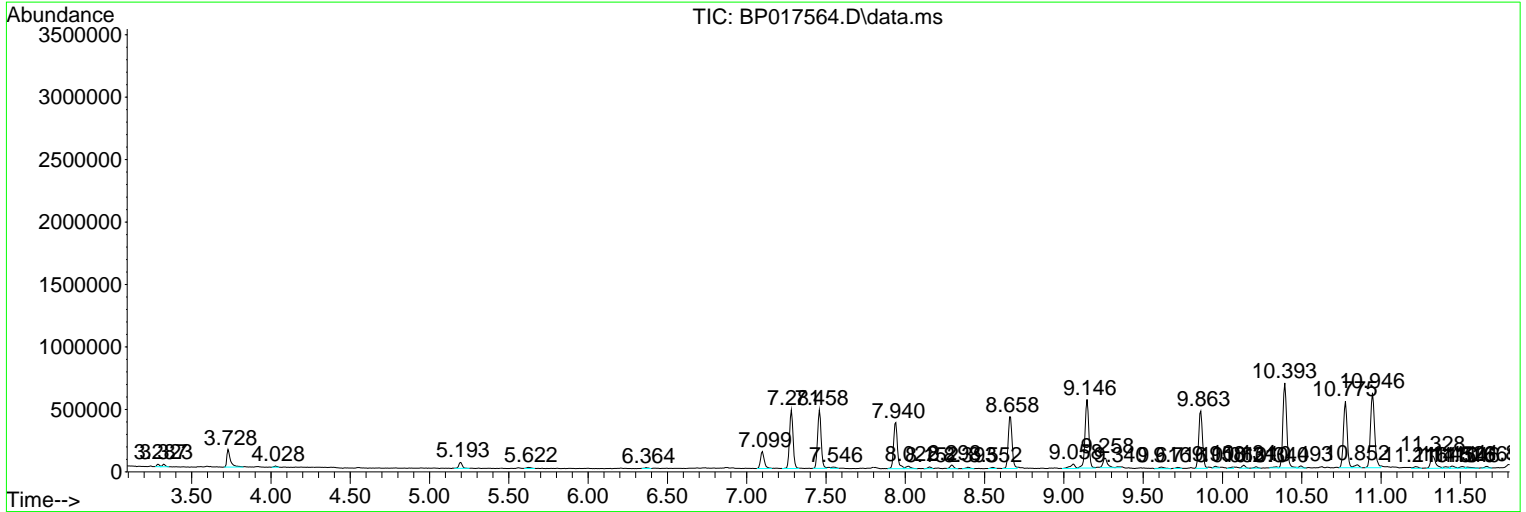
Sum of corrected areas: 39766682

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
 Quant Title : SVOA CALIBRATION

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



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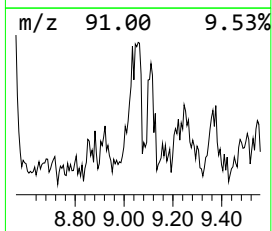
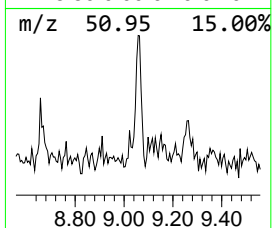
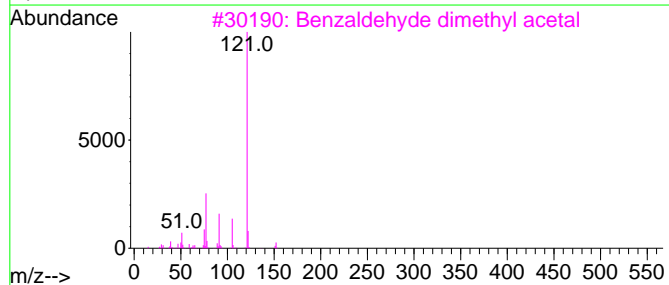
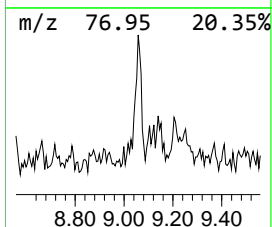
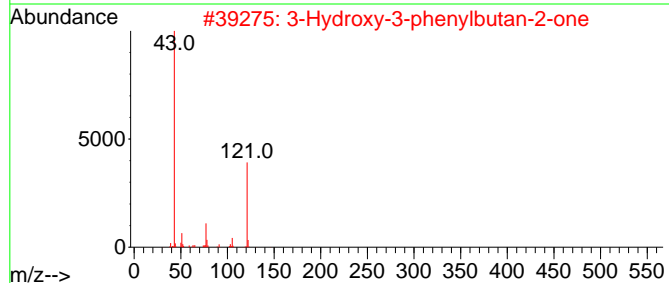
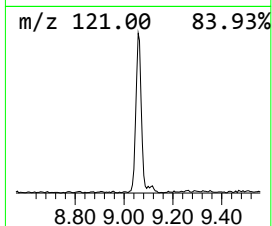
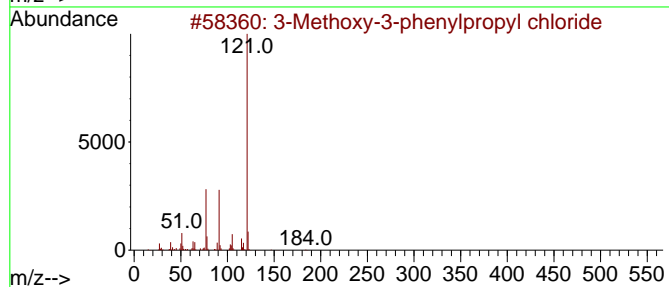
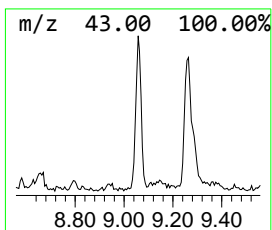
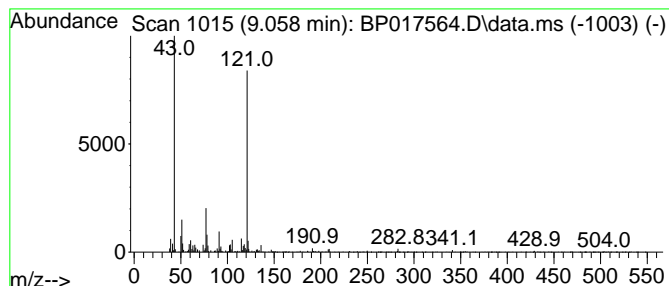
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100423.MA.M
 Quant Title : SVOA CALIBRATION

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

 Peak Number 2 3-Methoxy-3-phenylpropyl ch... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.058	2.71 ng/ul	84719	1,4-Dichlorobenzene-d4	7.940

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methoxy-3-phenylpropyl chloride	184	C10H13ClO	1000370-35-5	72
2		3-Hydroxy-3-phenylbutan-2-one	164	C10H12O2	003155-01-9	72
3		Benzaldehyde dimethyl acetal	152	C9H12O2	001125-88-8	64
4		d1-2-Phenyl-1,2-propanediol	152	C9H12O2	004217-66-7	64
5		Benzene, (1-methoxyethyl)-	136	C9H12O	004013-34-7	64



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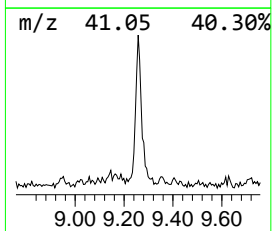
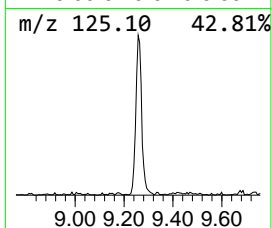
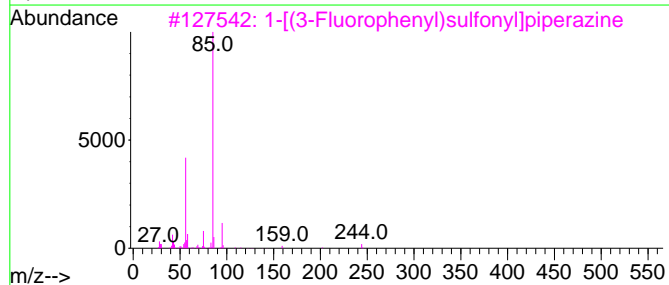
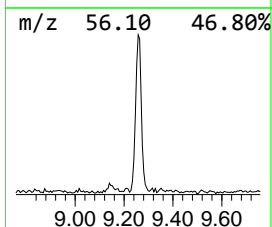
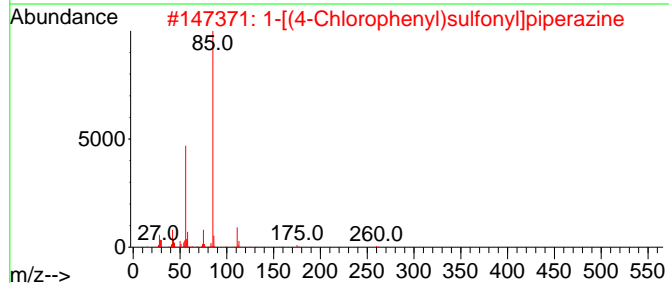
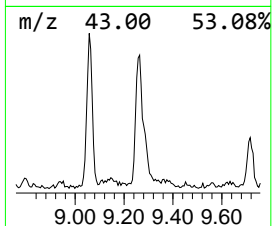
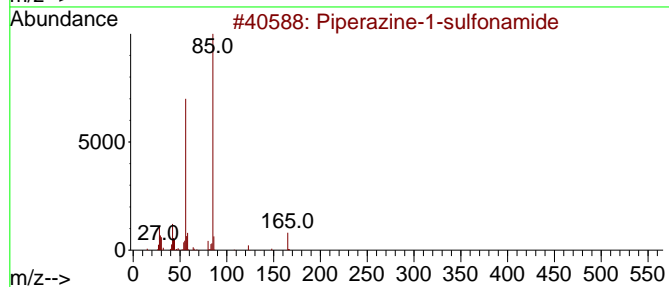
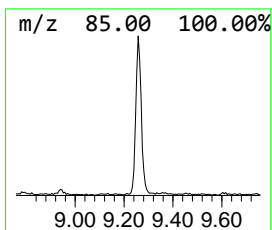
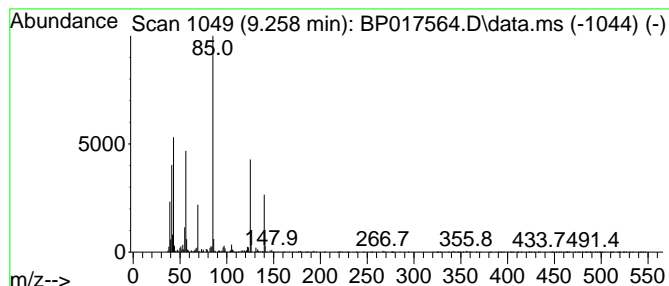
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TIC Library : C:\DATABASE\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.258	4.75 ng/ul	148461	1,4-Dichlorobenzene-d4	7.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Piperazine-1-sulfonamide	165	C4H11N3O2S	005906-30-9	47
2			1-[(4-Chlorophenyl)sulfonyl]pipe...	260	C10H13ClN2O2S	1000486-20-8	47
3			1-[(3-Fluorophenyl)sulfonyl]pipe...	244	C10H13FN2O2S	743441-88-5	47
4			1-[(4-Nitrophenyl)sulfonyl]piper...	271	C10H13N3O4S	403825-44-5	47
5			1-((3-chlorophenyl)sulfonyl)pipe...	260	C10H13ClN2O2S	233261-85-3	47



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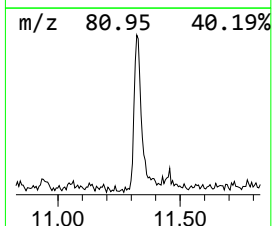
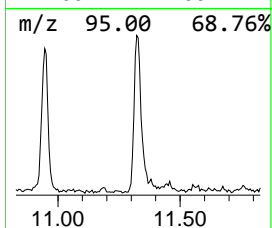
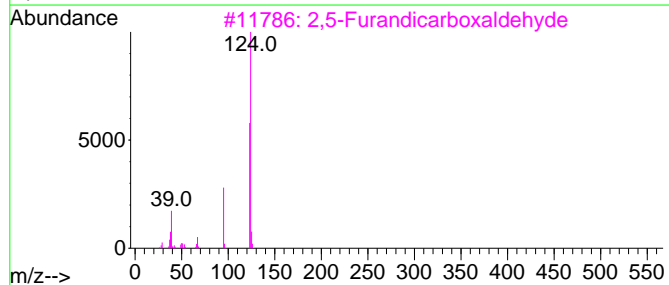
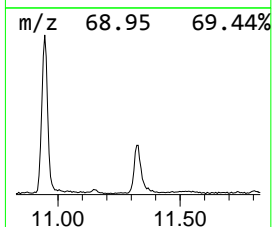
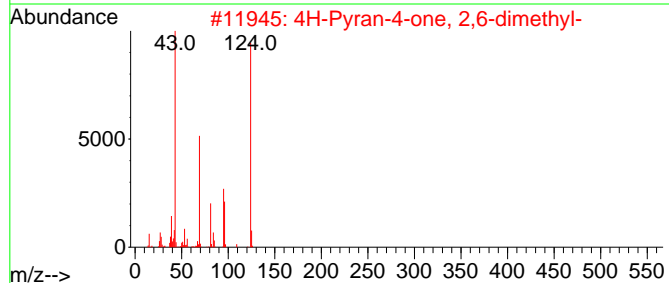
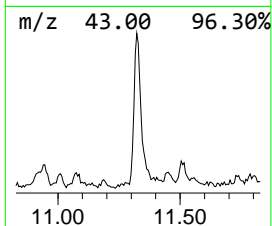
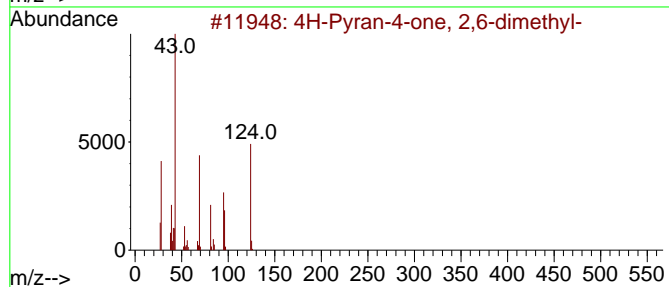
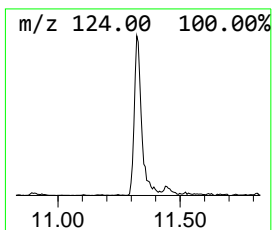
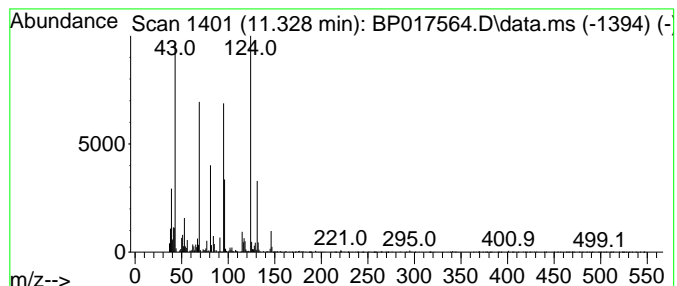
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 4 4H-Pyran-4-one, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.328	5.08 ng/ul	221208	Naphthalene-d8	10.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	70
2			4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	49
3			2,5-Furandicarboxaldehyde	124	C6H4O3	000823-82-5	40
4			5-Methyl-2-pyrazinylmethanol	124	C6H8N2O	061892-95-3	40
5			4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
 Acq On : 05 Oct 2023 14:14
 Operator : MA/JU
 Sample : 04679-09
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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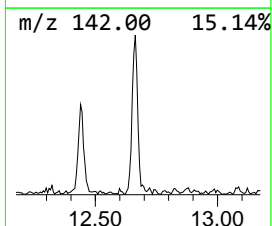
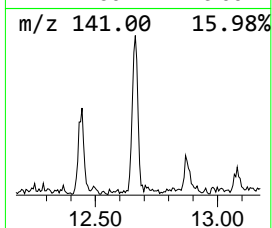
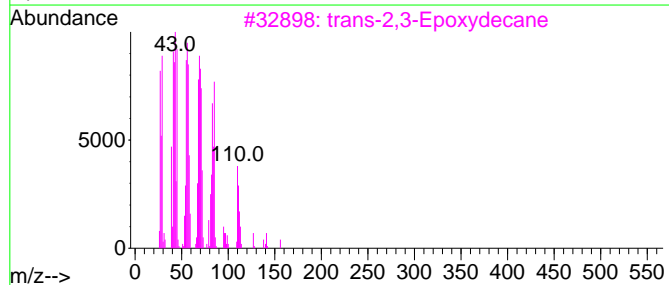
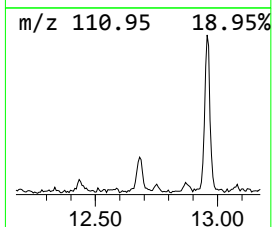
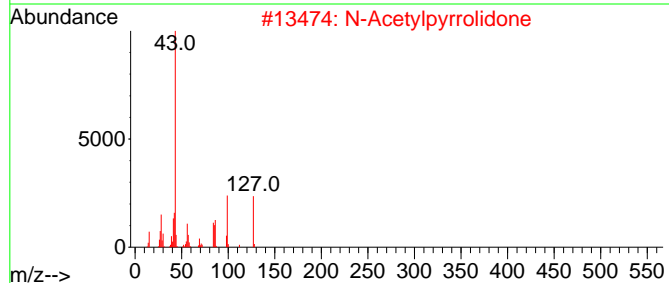
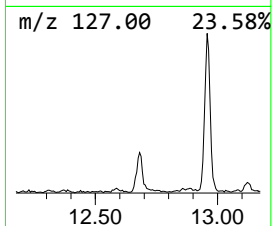
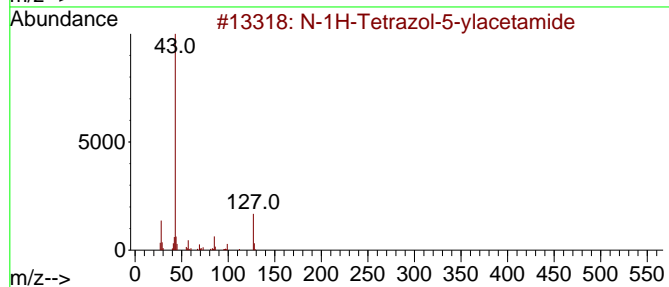
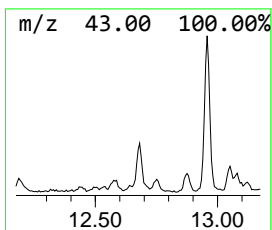
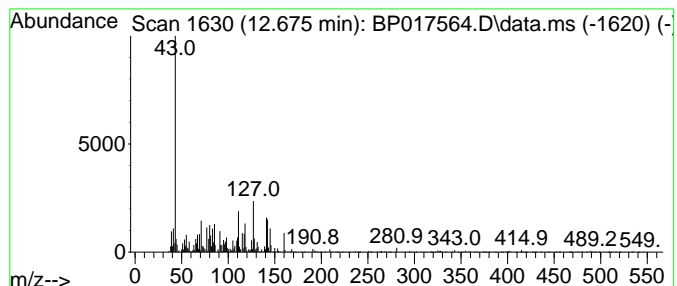
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 5 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.675	3.18 ng/ul	138596	Naphthalene-d8	10.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-1H-Tetrazol-5-ylacetamide	127	C3H5N5O	006158-77-6	14
2			N-Acetylpyrrolidone	127	C6H9NO2	000932-17-2	14
3			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	10
4			Urea, N-(2-chlorophenyl)-N'-methyl-	184	C8H9ClN2O	015500-96-6	10
5			Threose triacetate	246	C10H14O7	1000129-80-9	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
 Acq On : 05 Oct 2023 14:14
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 Sample : 04679-09
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 PMW-3(2030927)

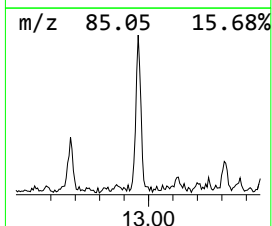
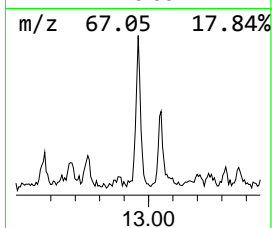
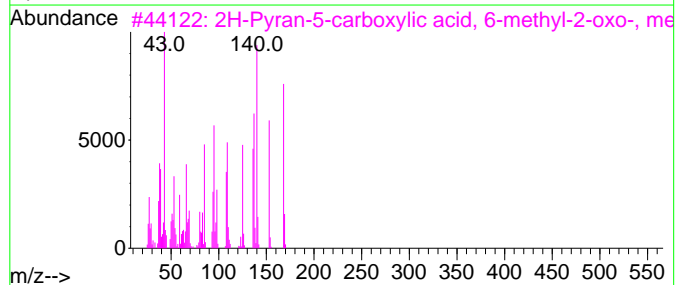
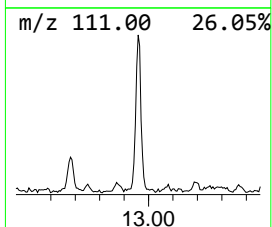
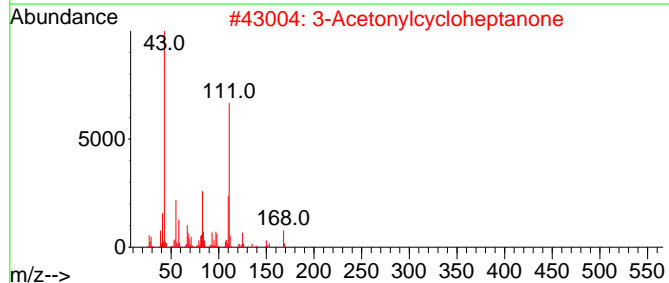
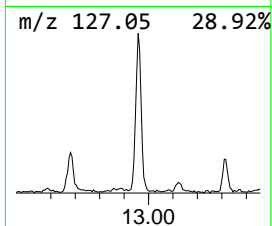
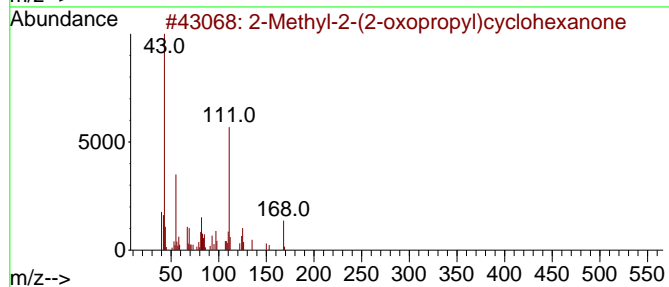
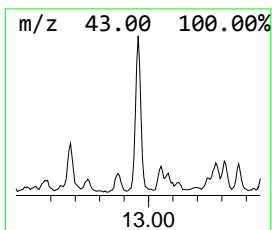
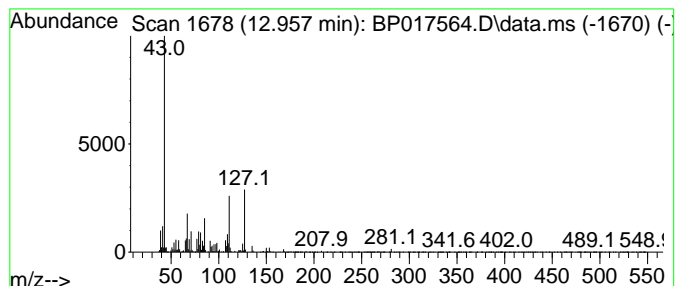
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 6 unknown-03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.957	4.13 ng/ul	248142	Acenaphthene-d10	14.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-2-(2-oxopropyl)cyclohex...	168	C10H16O2	1000427-09-9	32
2			3-Acetylcycloheptanone	168	C10H16O2	066921-76-4	12
3			2H-Pyran-5-carboxylic acid, 6-me...	168	C8H8O4	000669-40-9	10
4			5-Isopropyl-6-methyl-hepta-3,5-d...	168	C11H20O	1010187-77-8	10
5			N-Acetylpyrrolidone	127	C6H9NO2	000932-17-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
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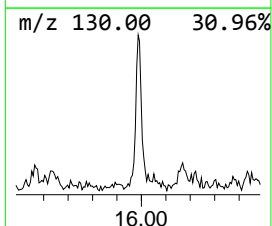
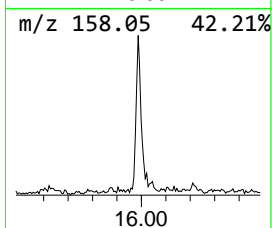
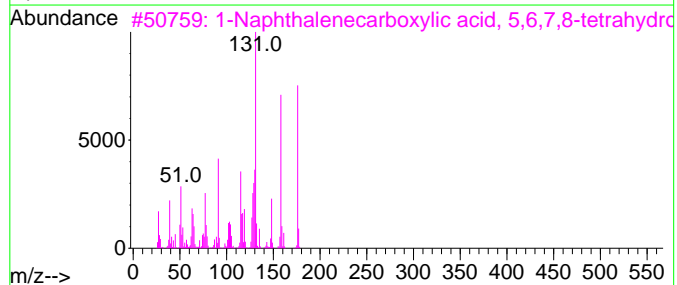
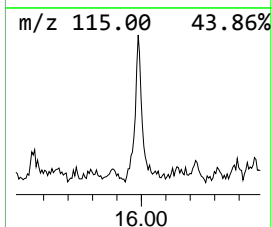
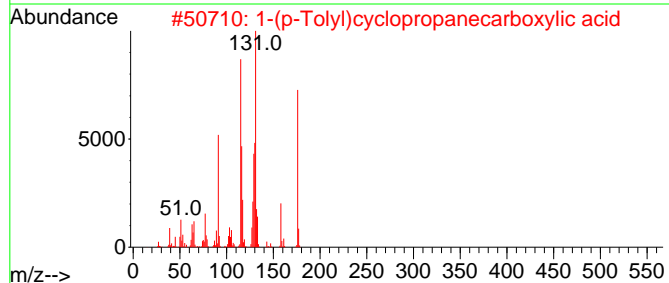
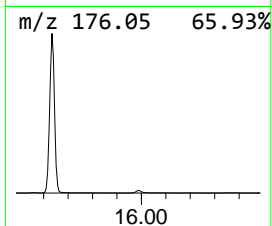
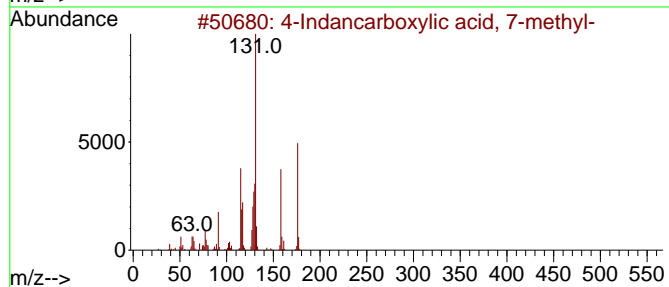
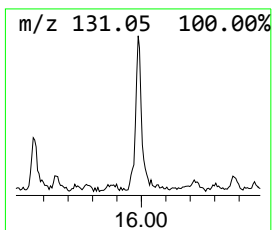
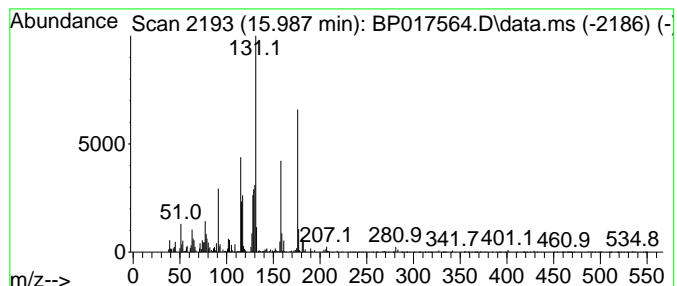
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 7 4-Indancarboxylic acid, 7-m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.987	2.76 ng/ul	165981	Acenaphthene-d10	14.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Indancarboxylic acid, 7-methyl-	176	C11H12O2	071042-74-5	98
2			1-(p-Tolyl)cyclopropanecarboxyli...	176	C11H12O2	083846-66-6	64
3			1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	52
4			2,3-Dihydro-1H-inden-5-ylacetic ...	176	C11H12O2	005453-98-5	52
5			1,2,3,4-Tetrahydro-1-naphthalene...	164	C10H12S	103324-34-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
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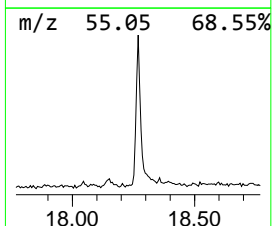
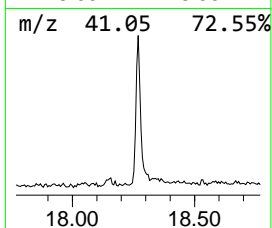
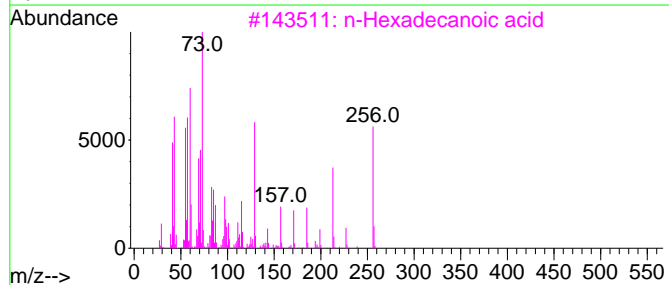
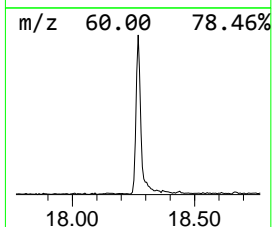
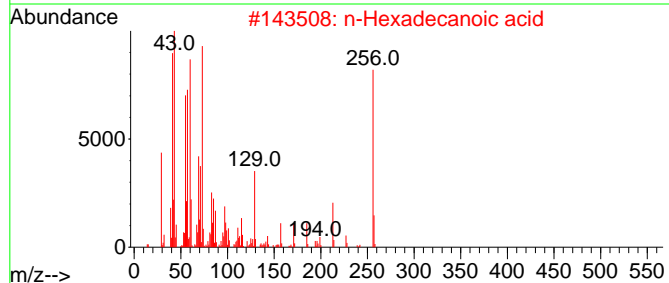
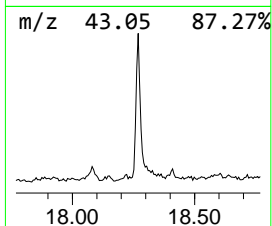
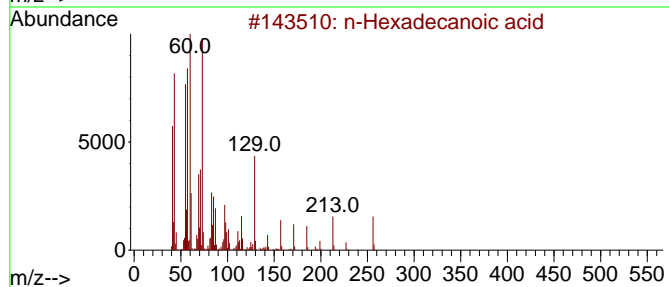
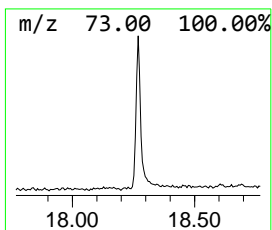
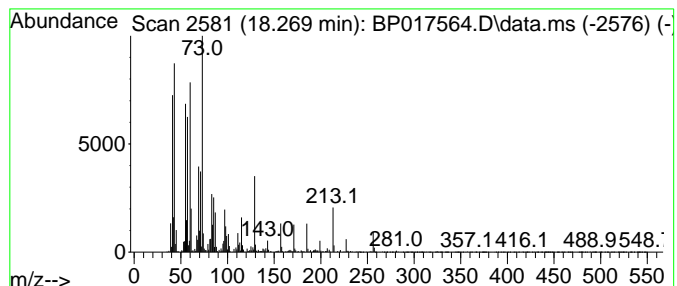
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 8 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.269	7.02 ng/ul	538999	Phenanthrene-d10	17.422

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	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
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 Misc :
 ALS Vial : 38 Sample Multiplier: 1

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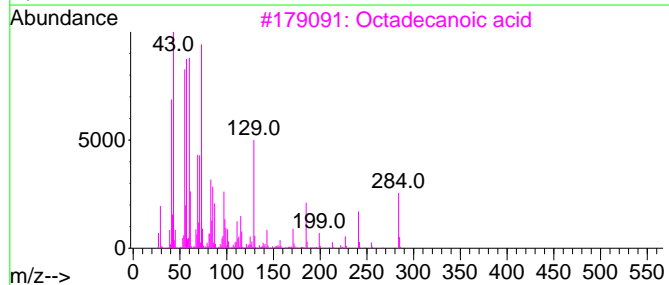
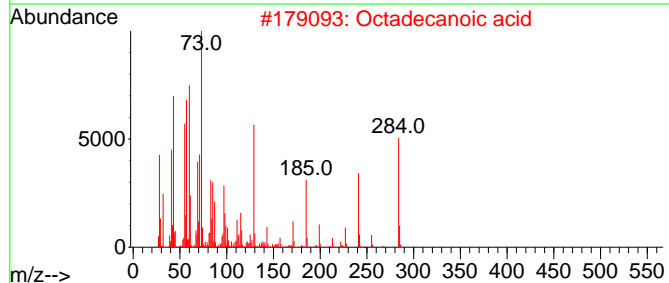
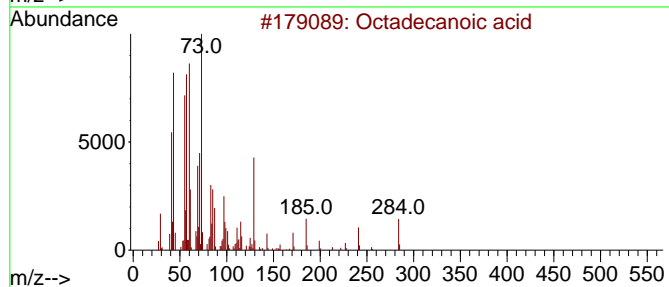
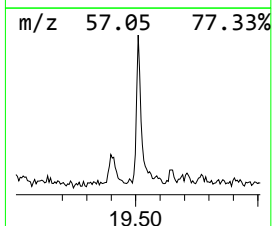
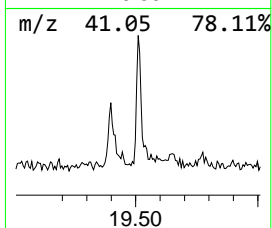
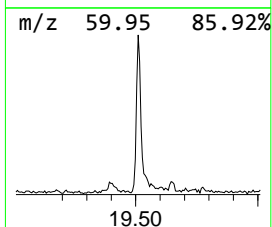
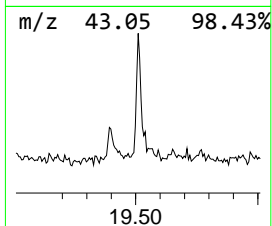
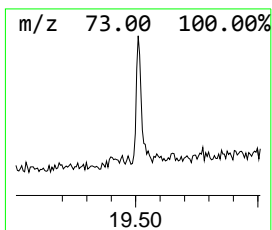
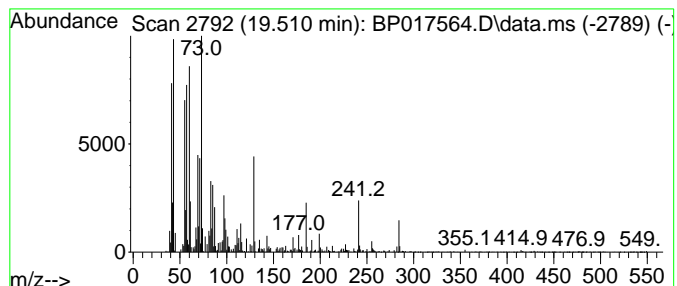
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	2.09 ng/ul	184827	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	94
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
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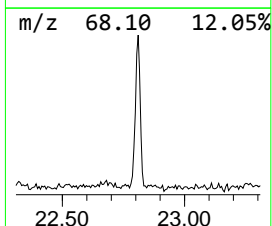
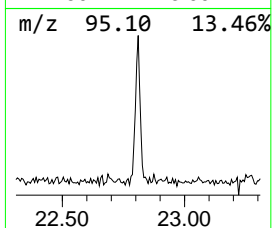
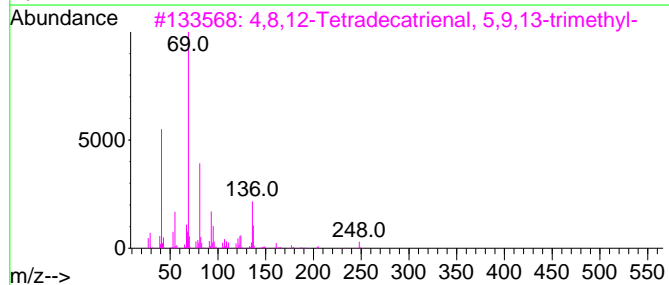
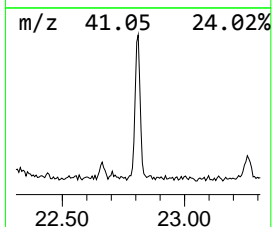
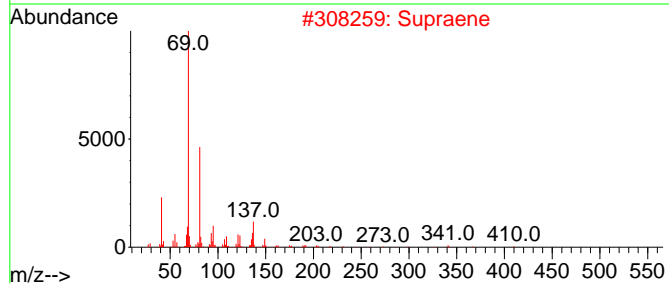
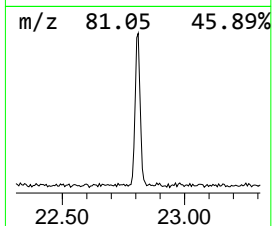
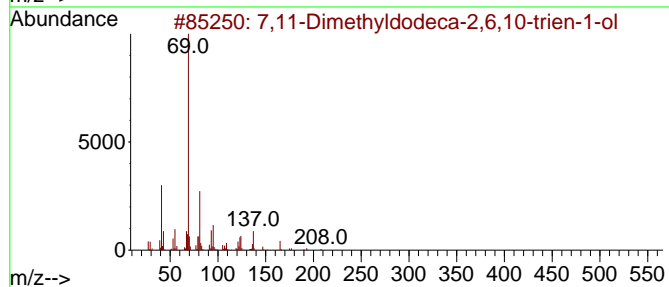
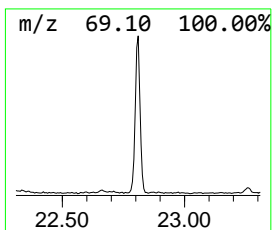
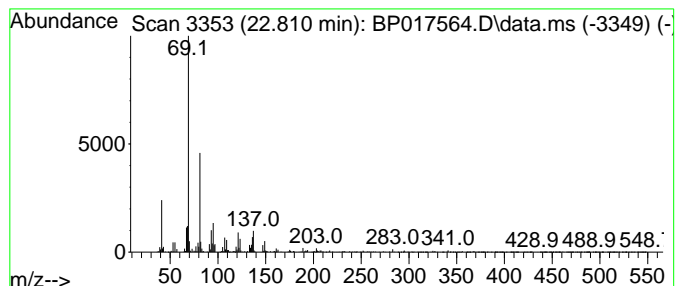
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 Quant Title : SVOA CALIBRATION

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

 Peak Number 10 7,11-Dimethyldodeca-2,6,10-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.810	3.78 ng/ul	334366	Chrysene-d12	21.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
2		Supraene	410	C30H50	007683-64-9	78
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100423\
 Data File : BP017564.D
 Acq On : 05 Oct 2023 14:14
 Operator : MA/JU
 Sample : 04679-09
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Methoxy-3-phe...	9.058	2.7	ng/u1	84719	1	7.940	625578	20.0
unknown-01	9.258	4.8	ng/u1	148461	1	7.940	625578	20.0
4H-Pyran-4-one, ...	11.328	5.1	ng/u1	221208	2	10.775	871436	20.0
unknown-02	12.675	3.2	ng/u1	138596	2	10.775	871436	20.0
unknown-03	12.957	4.1	ng/u1	248142	3	14.634	1200700	20.0
4-Indancarboxyl...	15.987	2.8	ng/u1	165981	3	14.634	1200700	20.0
n-Hexadecanoic ...	18.269	7.0	ng/u1	538999	4	17.422	1536420	20.0
Octadecanoic acid	19.510	2.1	ng/u1	184827	5	21.557	1770130	20.0
7,11-Dimethyldo...	22.810	3.8	ng/u1	334366	5	21.557	1770130	20.0