

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
 Data File : BP018383.D
 Acq On : 25 Nov 2023 23:48
 Operator : MA/JU
 Sample : 05261-10
 Misc :
 ALS Vial : 66 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCKQ9

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_P\Methods\SFAM-EPA-BP112223.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	10	14	24	rVB2	52466	89751	1.68%	0.102%
2	3.275	27	32	37	rVB	56138	77543	1.45%	0.088%
3	3.705	98	105	113	rBV2	103985	187185	3.50%	0.213%
4	3.805	117	122	127	rBV	249565	327679	6.13%	0.373%
5	3.881	132	135	139	rVV	53060	72054	1.35%	0.082%
6	3.934	139	144	150	rVB	55845	94130	1.76%	0.107%
7	4.022	155	159	165	rVB3	66967	93638	1.75%	0.107%
8	4.181	182	186	196	rBV	68275	103521	1.94%	0.118%
9	4.358	212	216	221	rBV	76799	97963	1.83%	0.112%
10	4.546	242	248	252	rBV2	17798	35349	0.66%	0.040%
11	4.593	252	256	261	rVV3	43542	64848	1.21%	0.074%
12	4.740	277	281	287	rVV4	24588	44225	0.83%	0.050%
13	4.840	294	298	303	rVB3	26929	40439	0.76%	0.046%
14	4.964	312	319	329	rVV2	281776	454238	8.50%	0.517%
15	5.052	329	334	339	rVV	66614	96461	1.80%	0.110%
16	5.846	462	469	477	rBV	161870	243075	4.55%	0.277%
17	6.293	541	545	551	rVV2	40450	64736	1.21%	0.074%
18	6.852	634	640	645	rBV4	20939	48454	0.91%	0.055%
19	7.028	659	670	673	rBV2	1045498	2736676	51.19%	3.115%
20	7.199	693	699	707	rVB	948940	1414773	26.46%	1.610%
21	7.393	725	732	740	rBV	1082186	1692054	31.65%	1.926%
22	7.463	740	744	756	rVB	97078	173805	3.25%	0.198%
23	7.863	805	812	820	rBV	1682546	2637234	49.33%	3.002%
24	8.105	844	853	860	rBV2	53806	94011	1.76%	0.107%
25	8.175	860	865	871	rVB7	23237	39138	0.73%	0.045%
26	8.316	883	889	894	rBV	39094	66184	1.24%	0.075%
27	8.575	922	933	941	rBV	390033	654301	12.24%	0.745%
28	8.687	943	952	963	rVV	2076537	3391234	63.43%	3.860%
29	8.805	966	972	988	rVB	455019	795604	14.88%	0.906%
30	9.022	1002	1009	1016	rBV	1007481	1645234	30.77%	1.873%
31	9.134	1023	1028	1034	rVB	144685	219510	4.11%	0.250%
32	9.269	1045	1051	1058	rVV3	38945	65148	1.22%	0.074%
33	9.457	1079	1083	1089	rVB5	21249	35891	0.67%	0.041%
34	9.746	1124	1132	1139	rBV	741931	1212278	22.67%	1.380%
35	9.993	1149	1174	1187	rVV	983975	4121594	77.09%	4.691%
36	10.104	1187	1193	1205	rVV	799257	1361652	25.47%	1.550%

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37	10.222	1208	1213	1217	rVV	48840	101526	1.90%	0.116%
38	10.281	1217	1223	1230	rVV	1301317	2112117	39.50%	2.404%
39	10.346	1232	1234	1244	rVB7	18166	33180	0.62%	0.038%
40	10.540	1259	1267	1275	rBV8	23372	72178	1.35%	0.082%
41	10.663	1281	1288	1302	rVB	2304152	3781549	70.73%	4.304%
42	10.804	1302	1312	1320	rBV	69020	159217	2.98%	0.181%
43	11.199	1373	1379	1389	rBV	450355	748343	14.00%	0.852%
44	11.446	1416	1421	1435	rVB	336884	576888	10.79%	0.657%
45	11.557	1435	1440	1444	rBV2	24995	40093	0.75%	0.046%
46	11.699	1459	1464	1470	rBV3	36468	60651	1.13%	0.069%
47	11.810	1479	1483	1490	rVV7	17950	35172	0.66%	0.040%
48	12.022	1514	1519	1526	rVB	118996	196746	3.68%	0.224%
49	12.122	1529	1536	1540	rBV	28036	51831	0.97%	0.059%
50	12.251	1554	1558	1568	rVB4	37083	73821	1.38%	0.084%
51	12.634	1618	1623	1629	rBV4	27699	56847	1.06%	0.065%
52	12.934	1670	1674	1679	rVB	31867	44752	0.84%	0.051%
53	13.269	1724	1731	1737	rBV2	56646	98651	1.85%	0.112%
54	13.404	1747	1754	1761	rBV	217942	351206	6.57%	0.400%
55	13.675	1797	1800	1804	rBV	24218	32777	0.61%	0.037%
56	13.828	1820	1826	1831	rVB6	52233	90021	1.68%	0.102%
57	13.910	1834	1840	1850	rBV	2604007	3518229	65.80%	4.005%
58	14.193	1877	1888	1899	rBV	2753551	4211612	78.77%	4.794%
59	14.345	1906	1914	1919	rBV	16197	32627	0.61%	0.037%
60	14.498	1933	1940	1948	rVV	3450676	5028206	94.05%	5.723%
61	14.575	1948	1953	1959	rVB10	21636	45633	0.85%	0.052%
62	14.687	1966	1972	1980	rBV	649309	945772	17.69%	1.077%
63	14.757	1982	1984	1990	rVV7	28675	46752	0.87%	0.053%
64	14.840	1991	1998	2004	rVV	177398	312845	5.85%	0.356%
65	14.916	2007	2011	2019	rVV6	56051	97707	1.83%	0.111%
66	15.487	2102	2108	2115	rBV	3660992	5208694	97.42%	5.929%
67	15.598	2121	2127	2136	rBV	523888	744781	13.93%	0.848%
68	15.987	2188	2193	2199	rVB6	32923	60033	1.12%	0.068%
69	16.075	2201	2208	2212	rBV2	25256	48973	0.92%	0.056%
70	16.710	2311	2316	2319	rBV	41303	59232	1.11%	0.067%
71	16.792	2326	2330	2338	rVB	58428	96773	1.81%	0.110%
72	17.122	2382	2386	2394	rBV2	33113	55496	1.04%	0.063%
73	17.245	2401	2407	2413	rBV	3704773	5153320	96.39%	5.866%
74	17.345	2418	2424	2434	rVV	2888770	4189686	78.36%	4.769%
75	17.428	2435	2438	2445	rVB8	21523	46256	0.87%	0.053%
76	17.751	2489	2493	2499	rBV	78413	103926	1.94%	0.118%

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77	17.933	2520	2524	2529	rBV2	76410	98014	1.83%	0.112%
78	18.016	2533	2538	2545	rVV	101907	142416	2.66%	0.162%
79	18.145	2555	2560	2567	rBV	577311	813370	15.21%	0.926%
80	18.204	2568	2570	2577	rVV2	66887	97734	1.83%	0.111%
81	18.292	2583	2585	2590	rVB4	26464	32135	0.60%	0.037%
82	18.451	2606	2612	2620	rBV2	71131	138620	2.59%	0.158%
83	18.598	2634	2637	2642	rBV2	76328	101728	1.90%	0.116%
84	18.657	2644	2647	2650	rVV	63039	79833	1.49%	0.091%
85	18.692	2650	2653	2659	rVB	352346	453955	8.49%	0.517%
86	18.839	2674	2678	2680	rBV3	25271	32541	0.61%	0.037%
87	18.916	2686	2691	2695	rBV	584893	713840	13.35%	0.813%
88	18.957	2695	2698	2703	rBV	122783	159890	2.99%	0.182%
89	19.069	2709	2717	2720	rBV5	144366	301170	5.63%	0.343%
90	19.386	2767	2771	2778	rBV	288037	398970	7.46%	0.454%
91	19.586	2799	2805	2814	rBV	3975973	5252678	98.25%	5.979%
92	19.757	2831	2834	2840	rVB2	54463	93824	1.75%	0.107%
93	19.886	2853	2856	2861	rVB	107247	124513	2.33%	0.142%
94	19.933	2862	2864	2870	rVV5	38793	55983	1.05%	0.064%
95	20.004	2873	2876	2883	rVB5	75045	119944	2.24%	0.137%
96	20.922	3028	3032	3036	rBV	174198	221962	4.15%	0.253%
97	21.092	3057	3061	3066	rBV	323979	455282	8.52%	0.518%
98	21.357	3101	3106	3111	rBV	3681704	4689889	87.72%	5.338%
99	23.639	3487	3494	3511	rVB2	2227716	4612058	86.26%	5.250%
100	23.798	3514	3521	3531	rVB	2572144	5346460	100.00%	6.086%

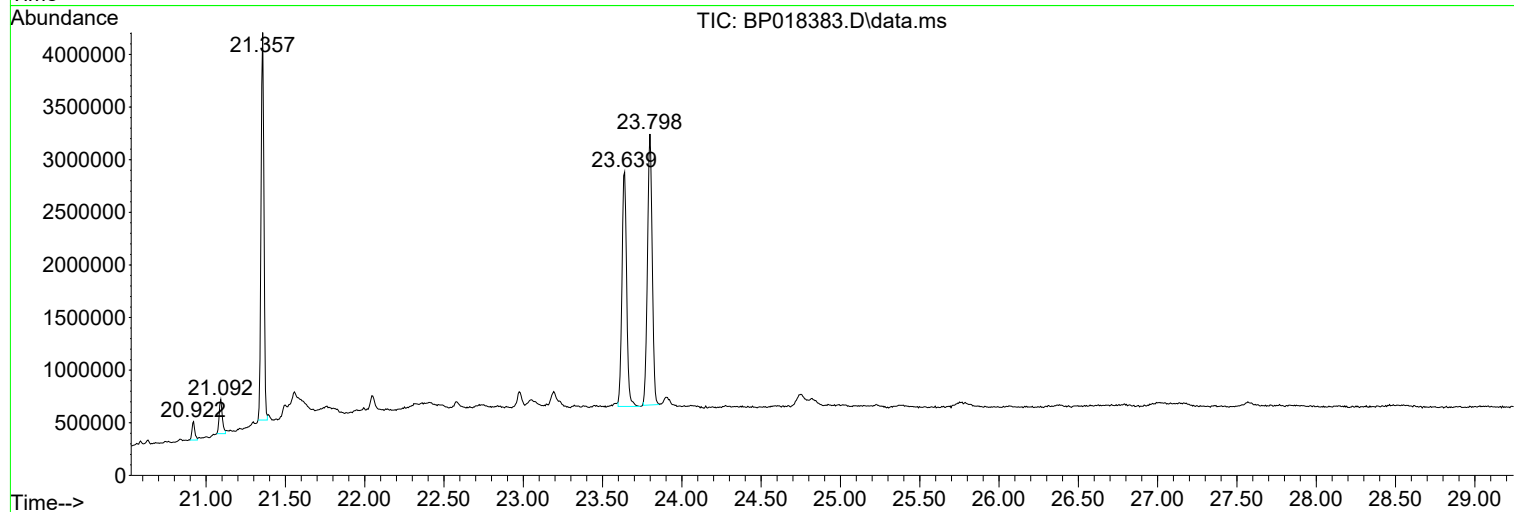
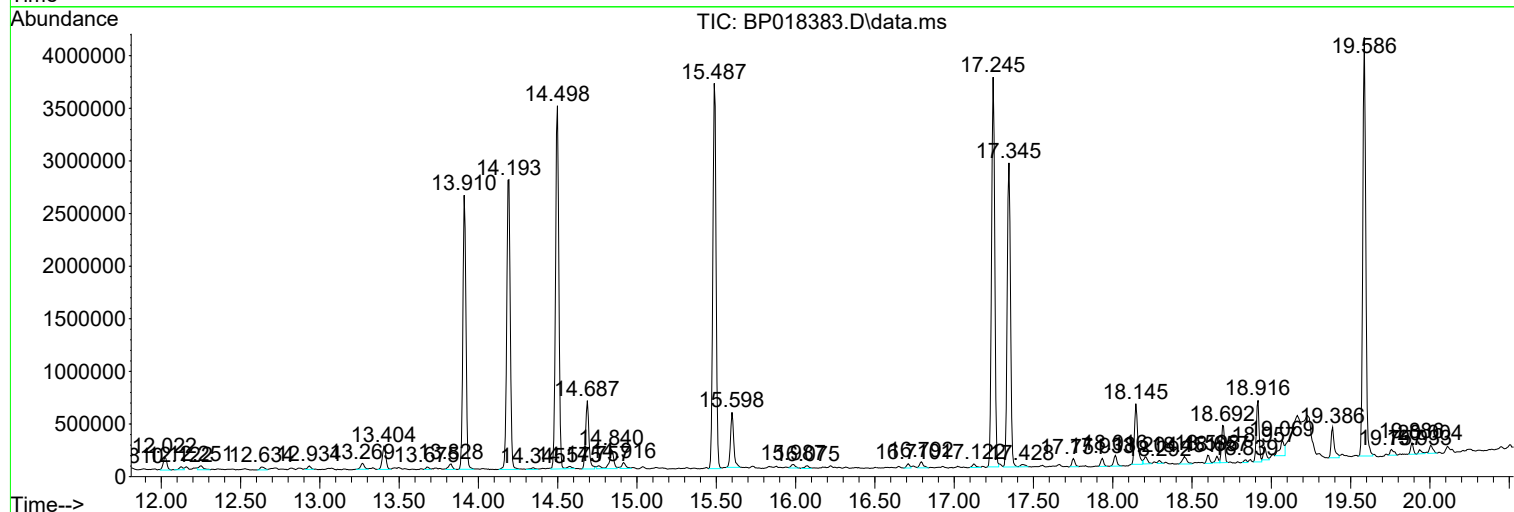
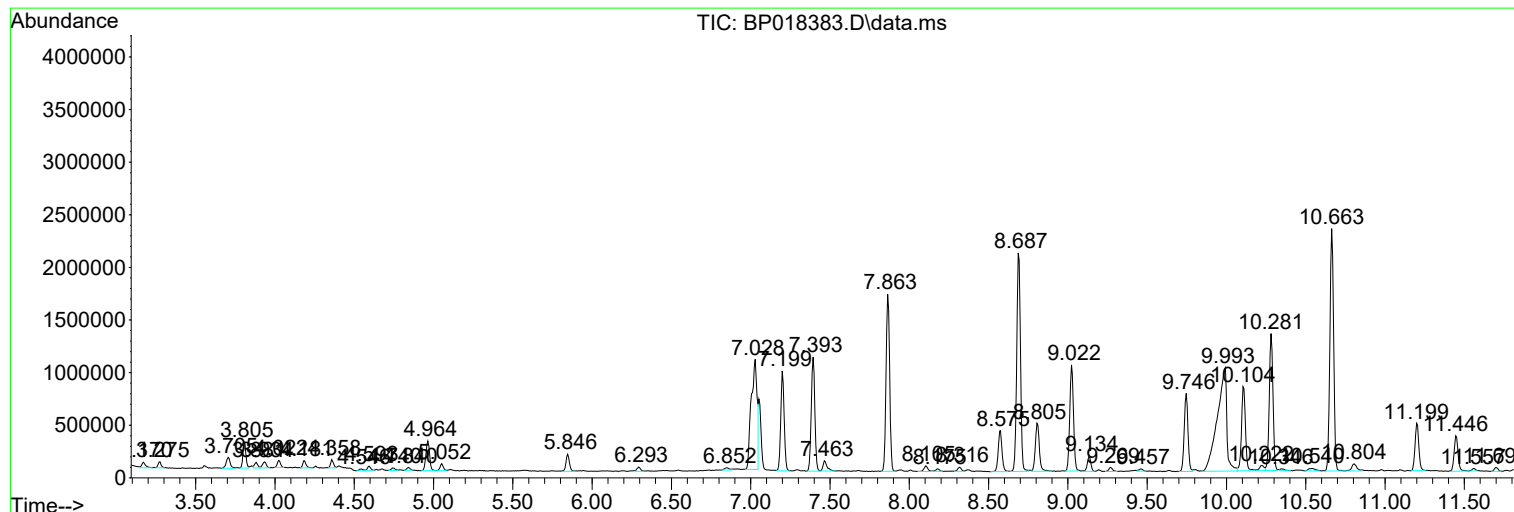
Sum of corrected areas: 87852538

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
Quant Title : SVOA CALIBRATION

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



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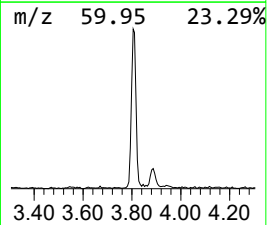
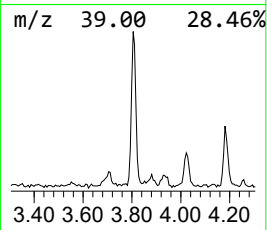
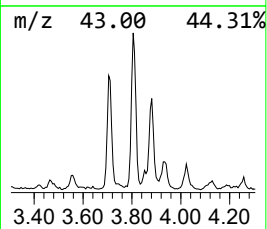
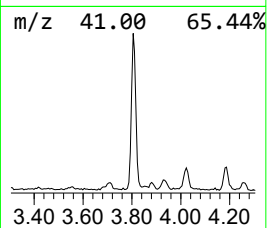
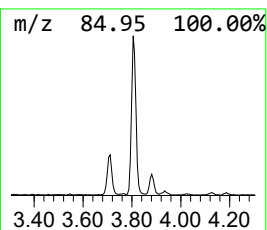
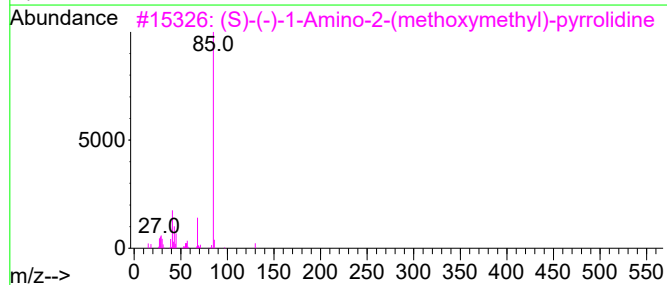
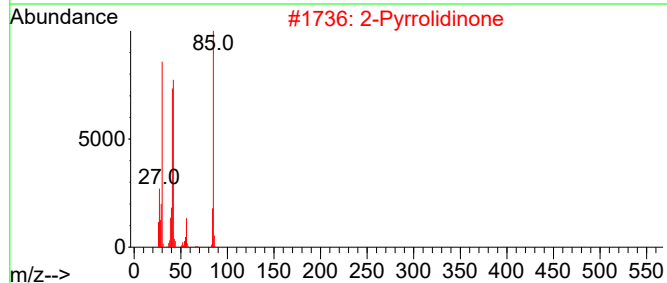
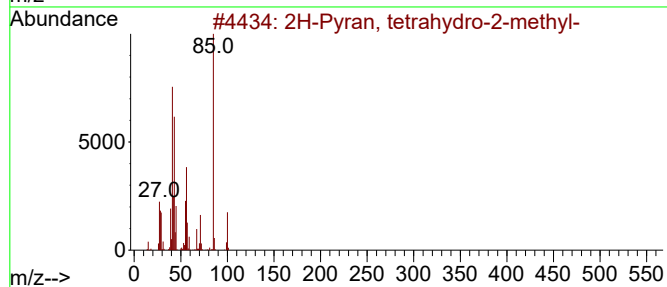
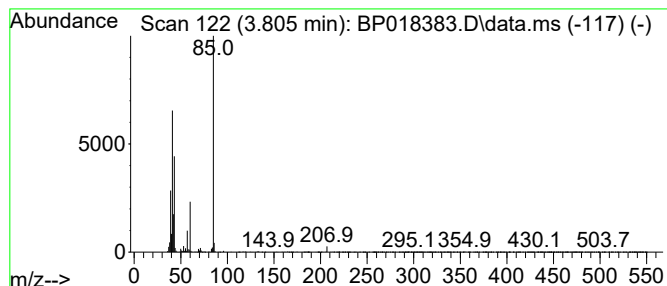
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.805	2.49 ng/ul	327679	1,4-Dichlorobenzene-d4	7.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	38
2	2-Pyrrolidinone			85	C4H7NO	000616-45-5	38
3	(S)-(-)-1-Amino-2-(methoxymethyl)pyrrolidine			130	C6H14N2O	059983-39-0	28
4	2-Pyrrolidinone			85	C4H7NO	000616-45-5	9
5	Pentanoic acid, propyl ester			144	C8H16O2	000141-06-0	9



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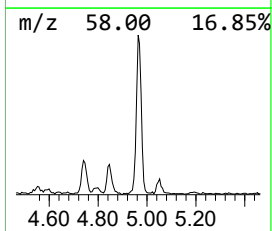
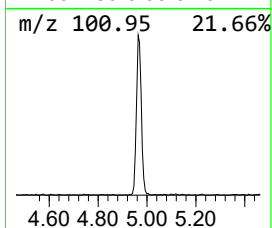
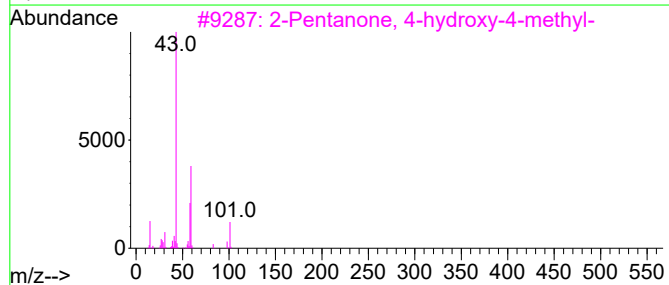
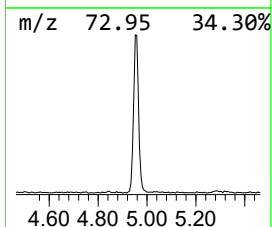
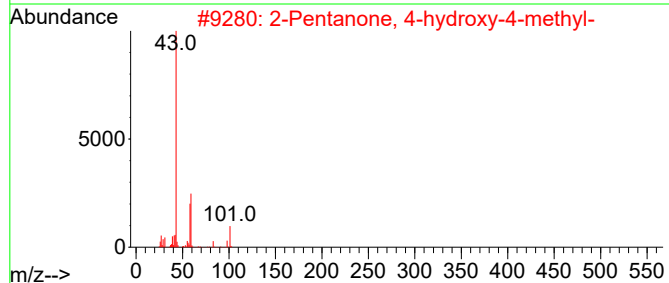
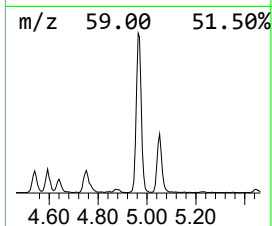
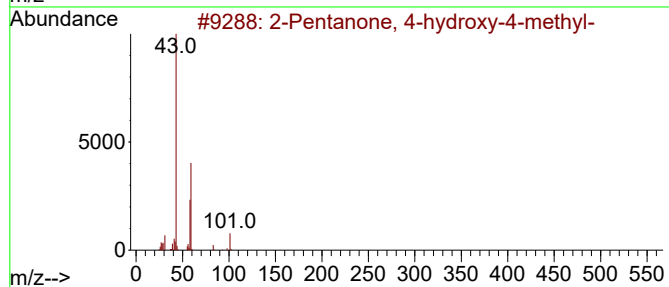
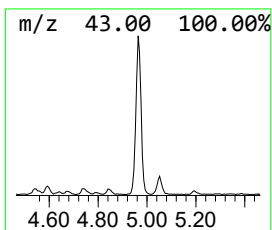
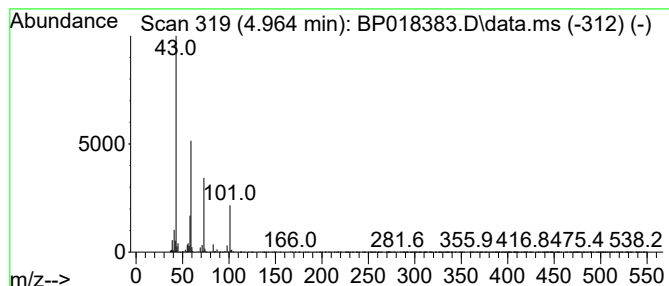
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.964	3.44 ng/ul	454238	1,4-Dichlorobenzene-d4	7.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	32
5	Butanamide	87	C4H9NO	000541-35-5	30



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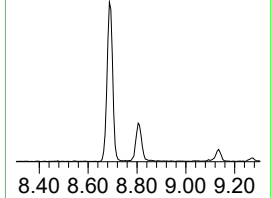
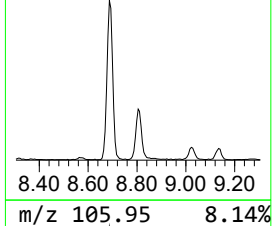
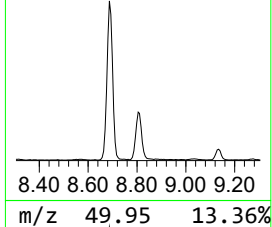
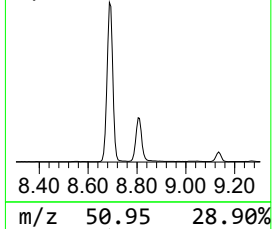
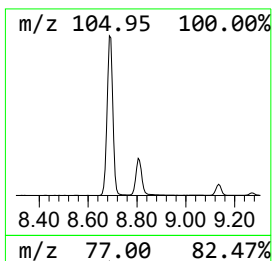
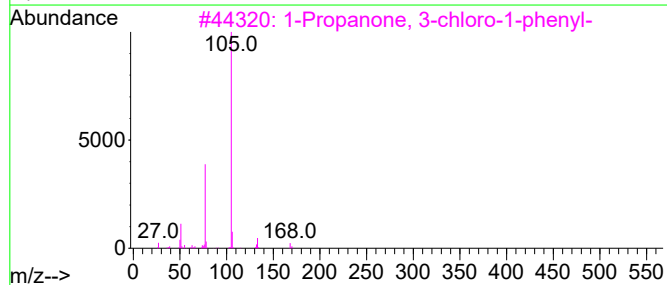
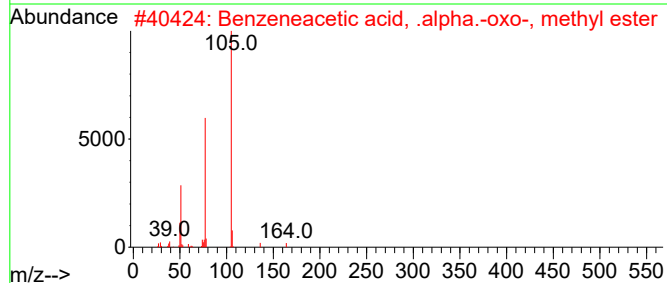
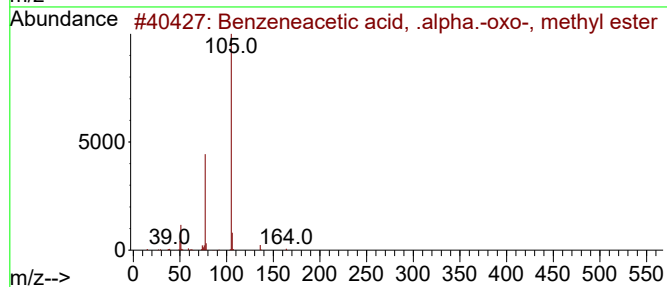
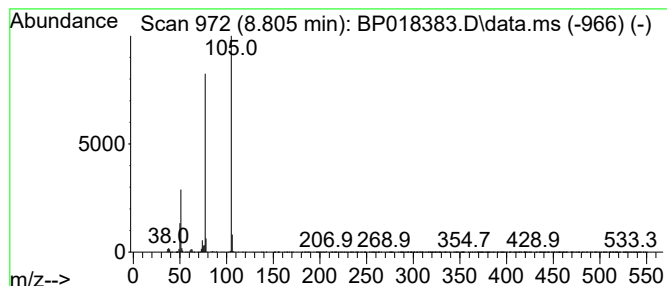
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzeneacetic acid, .alpha.... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.805	6.03 ng/ul	795604	1,4-Dichlorobenzene-d4	7.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	91
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	90
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	83
4			Benzoylformic acid	150	C8H6O3	000611-73-4	83
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018383.D
Acq On : 25 Nov 2023 23:48
Operator : MA/JU
Sample : 05261-10
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCKQ9

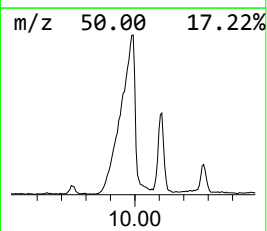
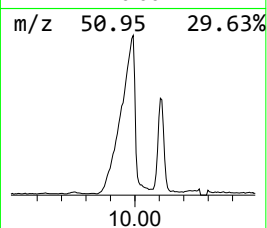
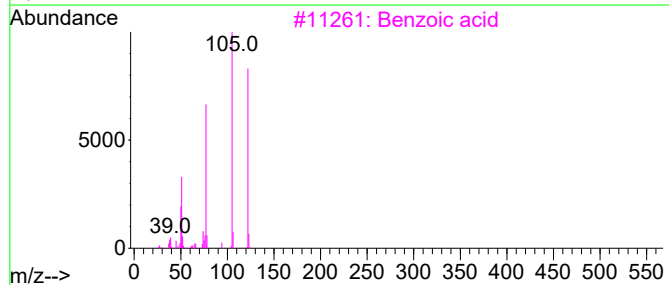
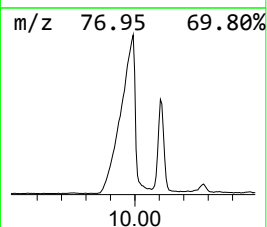
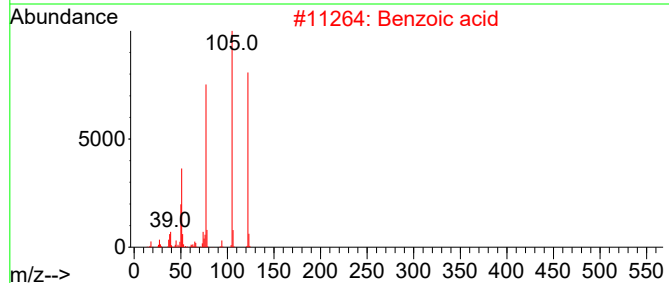
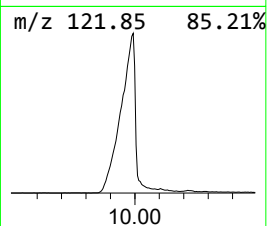
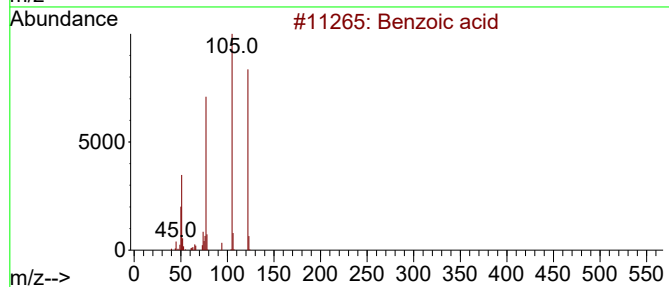
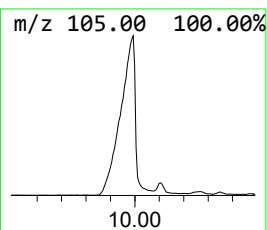
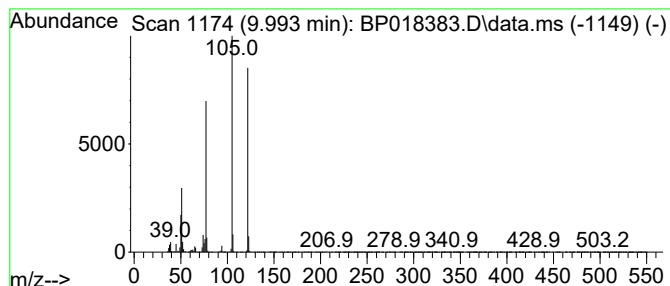
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Benzoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.993	21.80 ng/ul	4121590	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid			122	C7H6O2	000065-85-0	96
2	Benzoic acid			122	C7H6O2	000065-85-0	94
3	Benzoic acid			122	C7H6O2	000065-85-0	94
4	Benzoic acid			122	C7H6O2	000065-85-0	91
5	Benzoic acid, silver(1+) salt			228	C7H5AgO2	000532-31-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
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Misc :
ALS Vial : 66 Sample Multiplier: 1

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ClientSampleId :
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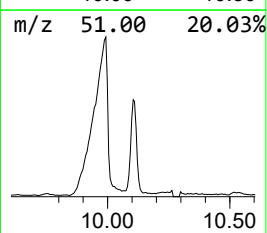
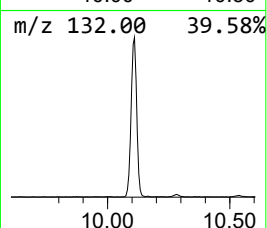
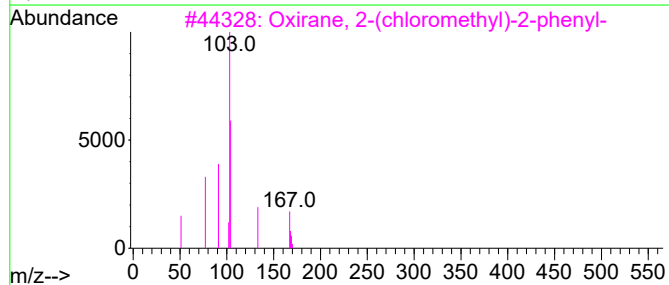
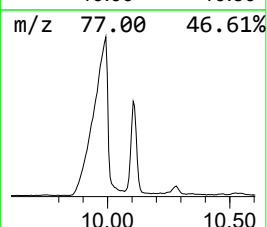
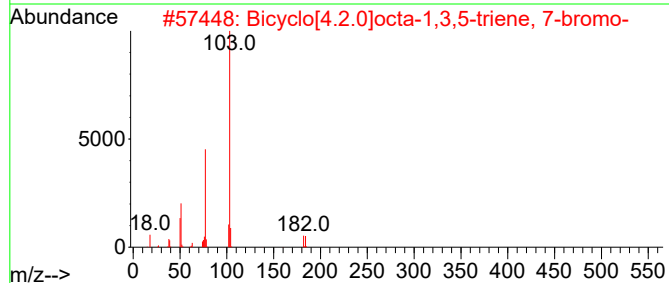
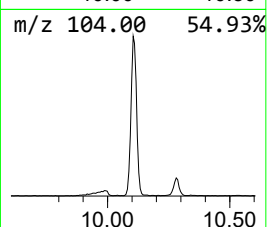
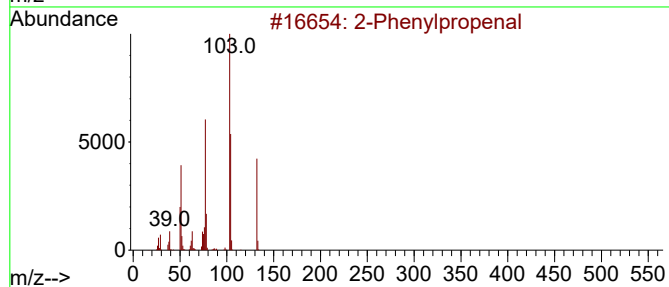
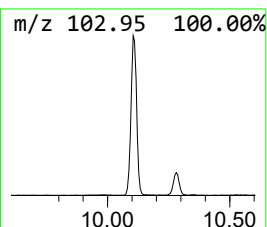
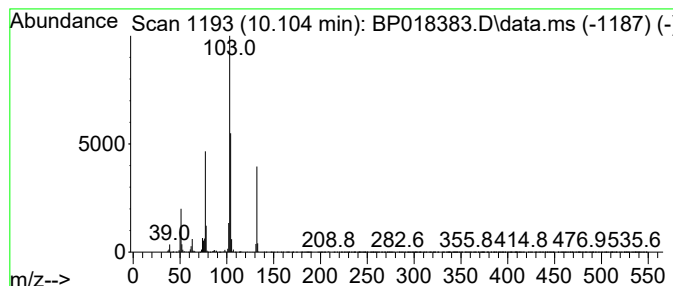
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 2-Phenylpropenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.105	7.20 ng/ul	1361650	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Phenylpropenal	132	C9H8O	004432-63-7	95
2			Bicyclo[4.2.0]octa-1,3,5-triene,...	182	C8H7Br	021120-91-2	47
3			Oxirane, 2-(chloromethyl)-2-phenyl-	168	C9H9ClO	001005-91-0	45
4			5(4H)-Isoxazolone, 3-phenyl-	161	C9H7NO2	001076-59-1	45
5			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018383.D
Acq On : 25 Nov 2023 23:48
Operator : MA/JU
Sample : 05261-10
Misc :
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ClientSampleId :
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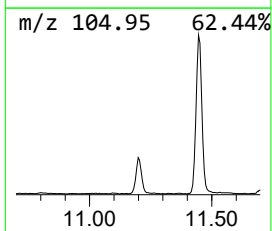
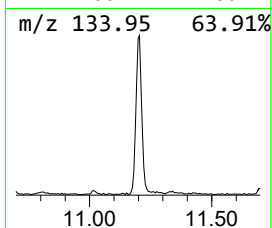
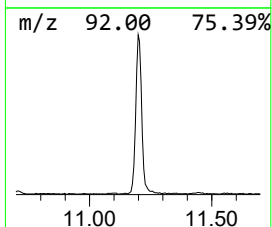
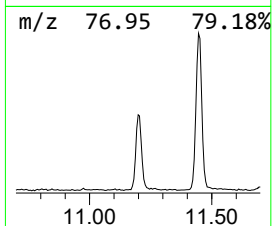
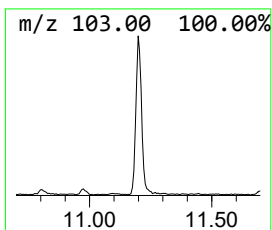
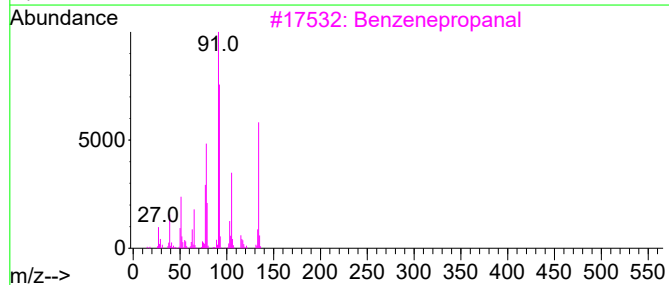
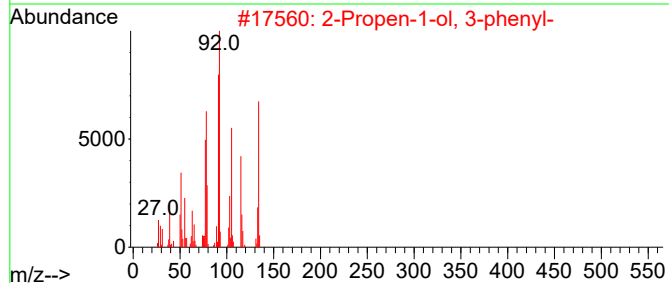
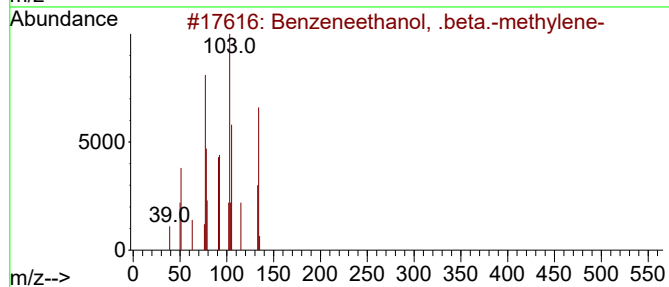
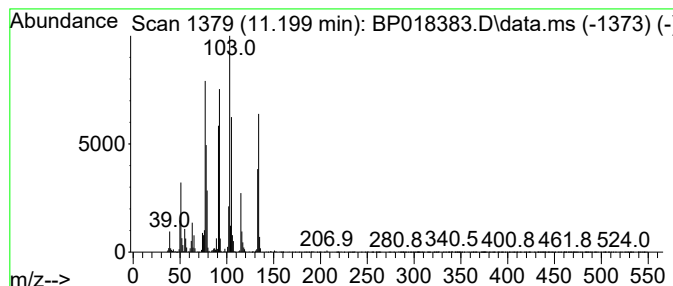
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Benzeneethanol, .beta.-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.199	3.96 ng/ul	748343	Naphthalene-d8	10.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzeneethanol, .beta.-methylene-	134	C9H10O	006006-81-1	90
2		2-Propen-1-ol, 3-phenyl-	134	C9H10O	000104-54-1	55
3		Benzenepropanal	134	C9H10O	000104-53-0	50
4		2-Propen-1-ol, 3-phenyl-	134	C9H10O	000104-54-1	49
5		2-Propen-1-ol, 3-phenyl-	134	C9H10O	000104-54-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018383.D
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Operator : MA/JU
Sample : 05261-10
Misc :
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Instrument :
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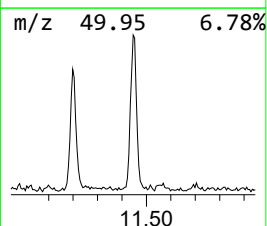
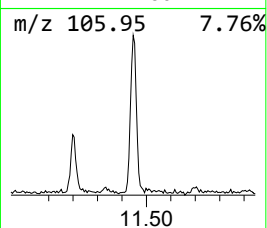
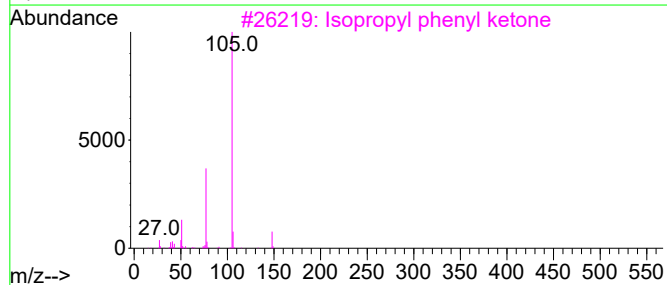
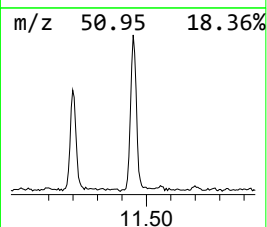
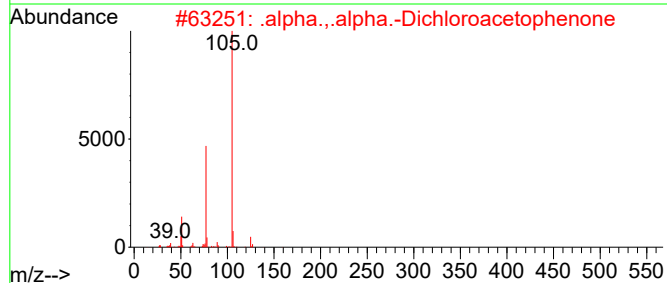
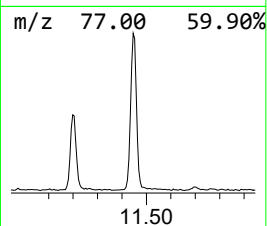
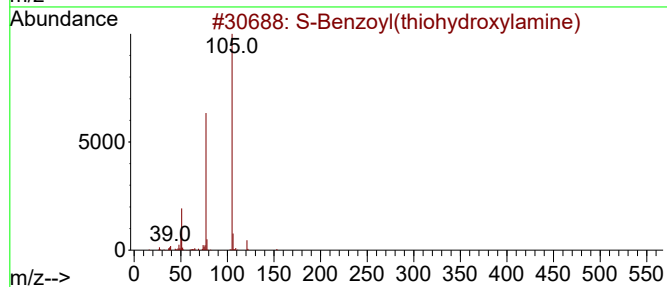
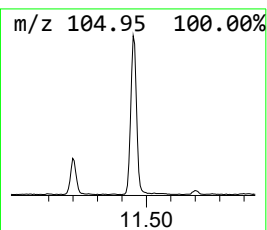
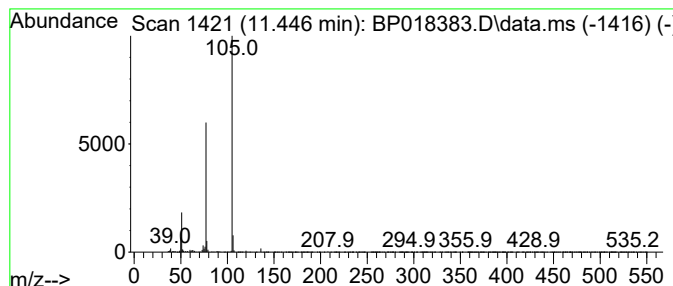
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 S-Benzoyl(thiohydroxylamine) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.446	3.05 ng/ul	576888	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			S-Benzoyl(thiohydroxylamine)	153	C7H7NO5	025740-80-1	78
2			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	78
3			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	78
4			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	78
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018383.D
Acq On : 25 Nov 2023 23:48
Operator : MA/JU
Sample : 05261-10
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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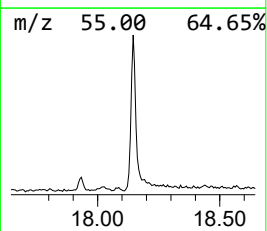
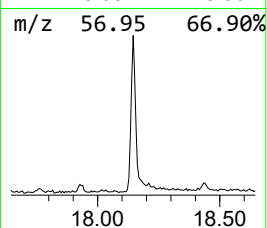
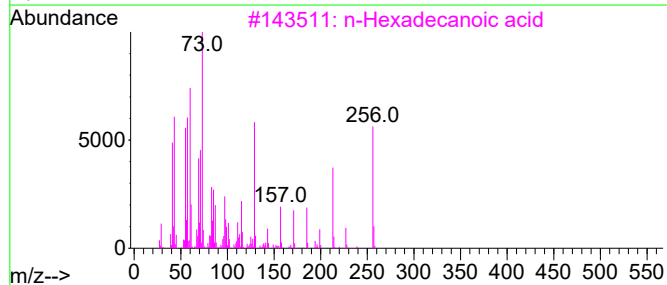
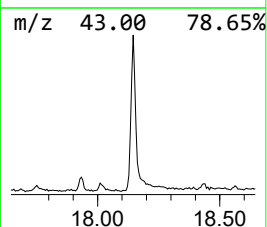
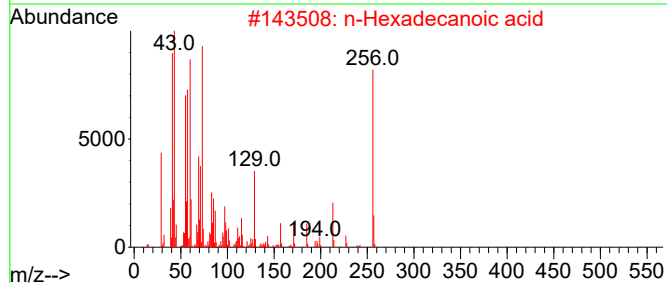
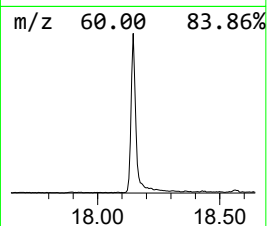
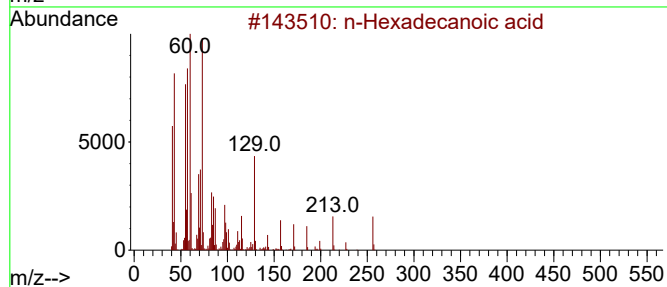
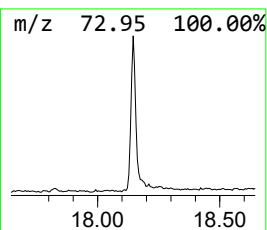
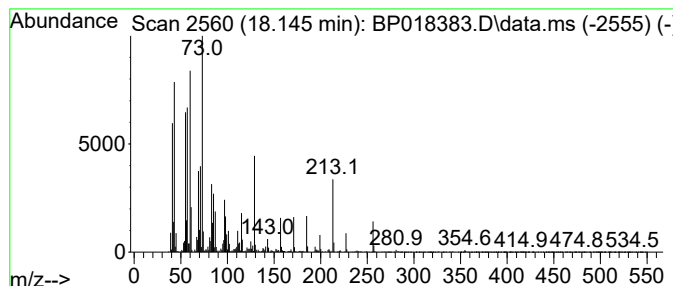
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	3.16 ng/ul	813370	Phenanthrene-d10	17.245

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	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			Tridecanoic acid	214	C13H26O2	000638-53-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018383.D
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Misc :
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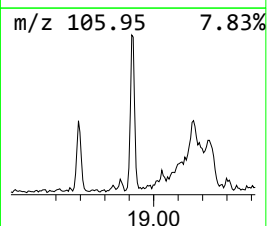
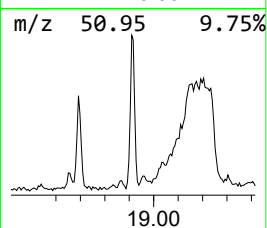
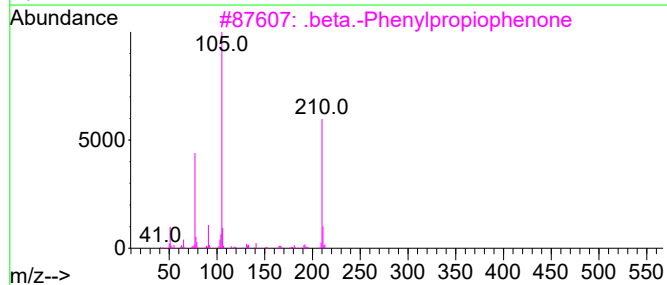
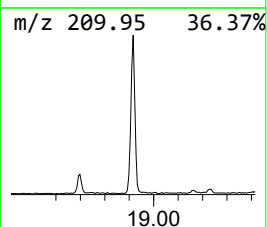
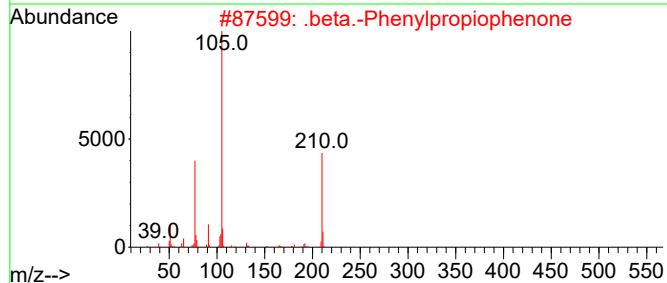
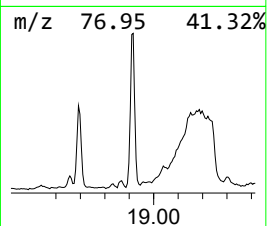
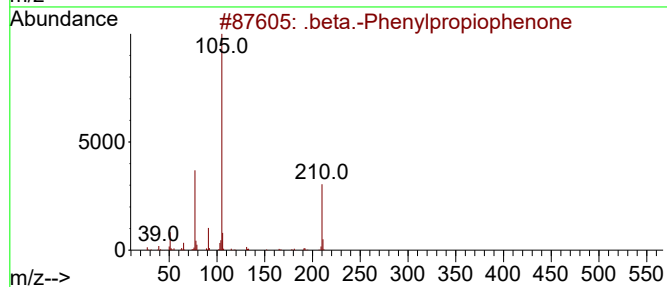
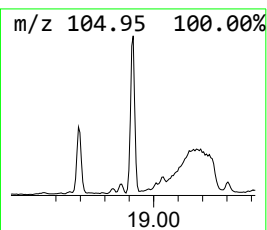
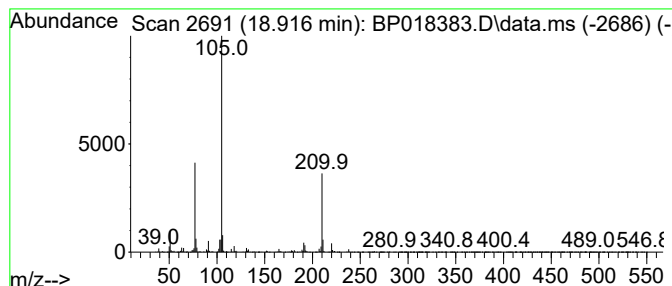
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 .beta.-Phenylpropiophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.916	2.77 ng/ul	713840	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	.beta.-Phenylpropiophenone	210	C15H14O	001083-30-3	93	
2	.	.beta.-Phenylpropiophenone	210	C15H14O	001083-30-3	93	
3	.	.beta.-Phenylpropiophenone	210	C15H14O	001083-30-3	87	
4	.	.beta.-Phenylpropiophenone	210	C15H14O	001083-30-3	87	
5	N-Benzoyl-3-phenylisoserine, 3-m...	383	C23H29NO4	1000453-74-7	72		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
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Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCKQ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
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
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2-Pentanone, 4-...	4.964	3.4	ng/ul	454238	1	7.863	2637230	20.0
Benzeneacetic a...	8.805	6.0	ng/ul	795604	1	7.863	2637230	20.0
Benzoic acid	9.993	21.8	ng/ul	4121590	2	10.663	3781550	20.0
2-Phenylpropenal	10.105	7.2	ng/ul	1361650	2	10.663	3781550	20.0
Benzeneethanol,...	11.199	4.0	ng/ul	748343	2	10.663	3781550	20.0
S-Benzoyl(thioh...	11.446	3.0	ng/ul	576888	2	10.663	3781550	20.0
n-Hexadecanoic ...	18.145	3.2	ng/ul	813370	4	17.245	5153320	20.0
.beta.-Phenylpr...	18.916	2.8	ng/ul	713840	4	17.245	5153320	20.0