

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
 Data File : BP014446.D
 Acq On : 31 Mar 2023 16:33
 Operator : CG/JU
 Sample : 02092-01
 Misc :
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CB964

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-BP032823.M
 Title : SVOA CALIBRATION

Signal : TIC: BP014446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.387	31	34	39	rBV	49141	56098	1.11%	0.101%
2	3.822	106	108	124	rBV	193984	314684	6.24%	0.569%
3	4.040	140	145	151	rVB2	16783	27302	0.54%	0.049%
4	4.146	158	163	168	rVB	16568	25444	0.50%	0.046%
5	4.258	177	182	186	rVB5	9933	16258	0.32%	0.029%
6	5.075	315	321	325	rBV	14653	23164	0.46%	0.042%
7	5.293	354	358	365	rVB2	23864	37354	0.74%	0.068%
8	6.393	539	545	550	rBV4	9541	15970	0.32%	0.029%
9	7.105	664	666	671	rVB4	4149	5197	0.10%	0.009%
10	7.175	671	678	691	rBV	193650	353686	7.01%	0.639%
11	7.334	698	705	716	rBV	783502	1260449	24.97%	2.279%
12	7.540	733	740	757	rBV	790769	1260662	24.98%	2.279%
13	7.869	791	796	799	rVB6	3520	5047	0.10%	0.009%
14	8.010	813	820	834	rBV	798147	1267541	25.12%	2.292%
15	8.728	934	942	957	rBV	627837	1110262	22.00%	2.007%
16	9.187	1013	1020	1035	rBV	1014146	1710165	33.89%	3.092%
17	9.540	1074	1080	1091	rVB3	78033	149807	2.97%	0.271%
18	9.816	1122	1127	1136	rVB10	13957	26558	0.53%	0.048%
19	9.916	1136	1144	1156	rBV	826253	1419598	28.13%	2.567%
20	10.199	1186	1192	1193	rBV6	3723	5933	0.12%	0.011%
21	10.387	1219	1224	1229	rBV8	4044	7159	0.14%	0.013%
22	10.457	1229	1236	1257	rBV	1074249	2039350	40.41%	3.687%
23	10.740	1281	1284	1288	rVB6	4091	5126	0.10%	0.009%
24	10.834	1293	1300	1308	rBV	1136984	1864612	36.95%	3.371%
25	10.981	1318	1325	1345	rBV	336395	720727	14.28%	1.303%
26	11.193	1355	1361	1370	rVB	6556	14678	0.29%	0.027%
27	11.663	1430	1441	1442	rBV	8041	17041	0.34%	0.031%
28	11.851	1469	1473	1476	rBV6	3864	7080	0.14%	0.013%
29	12.069	1504	1510	1512	rBV6	6074	10991	0.22%	0.020%
30	12.157	1520	1525	1530	rBV8	8531	14124	0.28%	0.026%
31	12.234	1533	1538	1543	rBV7	6560	12636	0.25%	0.023%
32	12.281	1544	1546	1552	rVB7	3796	5684	0.11%	0.010%
33	12.334	1552	1555	1558	rBV5	4260	6043	0.12%	0.011%
34	12.428	1565	1571	1576	rBV2	17951	33098	0.66%	0.060%
35	12.551	1590	1592	1597	rVB6	4791	5948	0.12%	0.011%
36	12.957	1658	1661	1666	rVB6	7864	11548	0.23%	0.021%

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37	13.010	1666	1670	1674	rBV6	6359	10949	0.22%	0.020%
38	13.128	1686	1690	1695	rVB7	7776	13365	0.26%	0.024%
39	13.275	1713	1715	1719	rVB5	6054	7109	0.14%	0.013%
40	13.387	1731	1734	1739	rBV6	6965	10450	0.21%	0.019%
41	13.463	1742	1747	1751	rBV7	14650	21965	0.44%	0.040%
42	13.545	1757	1761	1770	rVB4	15746	27617	0.55%	0.050%
43	13.663	1778	1781	1786	rVB7	10385	15658	0.31%	0.028%
44	13.987	1831	1836	1837	rBV5	5298	7076	0.14%	0.013%
45	14.069	1843	1850	1862	rBV	2279257	3271304	64.82%	5.914%
46	14.251	1880	1881	1886	rBV5	6045	7218	0.14%	0.013%
47	14.363	1893	1900	1913	rBV	2559528	3788016	75.06%	6.849%
48	14.616	1940	1943	1945	rBV	11455	11247	0.22%	0.020%
49	14.663	1945	1951	1959	rVB	1537855	2337794	46.32%	4.227%
50	14.910	1988	1993	2006	rBV3	58426	176210	3.49%	0.319%
51	15.481	2086	2090	2094	rBV2	21615	31631	0.63%	0.057%
52	15.663	2114	2121	2133	rBV	3124717	4514312	89.45%	8.162%
53	15.786	2136	2142	2152	rBV	1015292	1478896	29.30%	2.674%
54	15.869	2152	2156	2160	rVV	93639	113177	2.24%	0.205%
55	16.028	2177	2183	2196	rVB	549635	726045	14.39%	1.313%
56	16.181	2203	2209	2219	rBV	379036	533451	10.57%	0.964%
57	16.516	2263	2266	2269	rBV	16843	17754	0.35%	0.032%
58	16.604	2277	2281	2285	rVB6	12020	20193	0.40%	0.037%
59	16.692	2291	2296	2308	rBV	253306	417119	8.26%	0.754%
60	17.428	2415	2421	2431	rBV	1700247	2382071	47.20%	4.307%
61	17.528	2432	2438	2447	rBV	3066130	4318147	85.56%	7.807%
62	18.292	2564	2568	2575	rBV	217166	317019	6.28%	0.573%
63	18.704	2635	2638	2642	rVB2	41421	50587	1.00%	0.091%
64	19.333	2742	2745	2749	rBV2	38577	43843	0.87%	0.079%
65	19.522	2773	2777	2786	rBV2	96149	159871	3.17%	0.289%
66	19.757	2811	2817	2822	rBV	3602488	4725855	93.64%	8.544%
67	20.722	2979	2981	2986	rVB3	93852	106725	2.11%	0.193%
68	21.198	3059	3062	3068	rBV	174318	266060	5.27%	0.481%
69	21.516	3111	3116	3122	rBV	1696954	2234921	44.28%	4.041%
70	23.874	3509	3517	3528	rBV2	2446280	5046938	100.00%	9.125%
71	24.033	3538	3544	3558	rVB2	1214891	2561815	50.76%	4.632%
72	24.680	3648	3654	3663	rVB2	784707	1670882	33.11%	3.021%

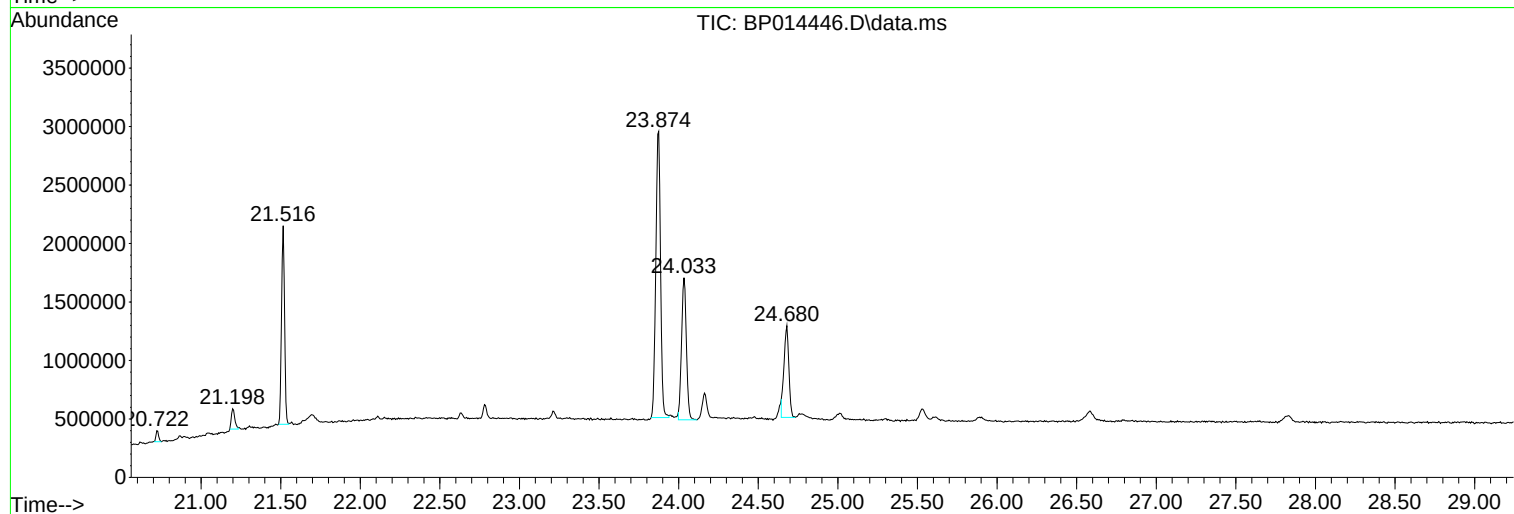
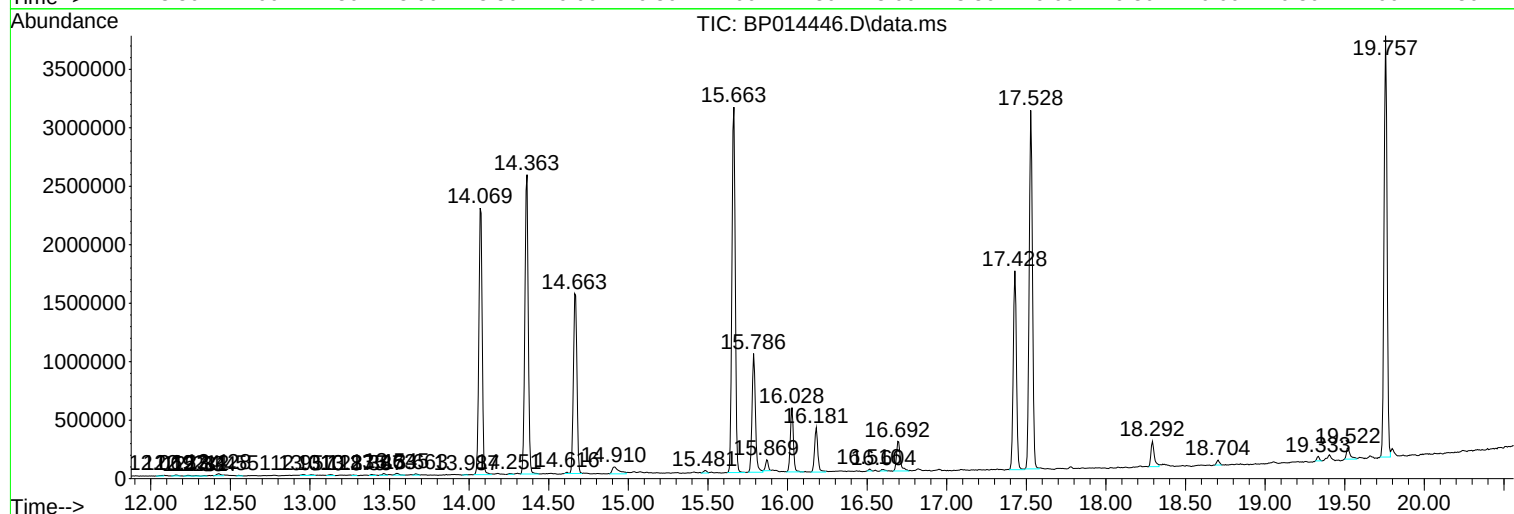
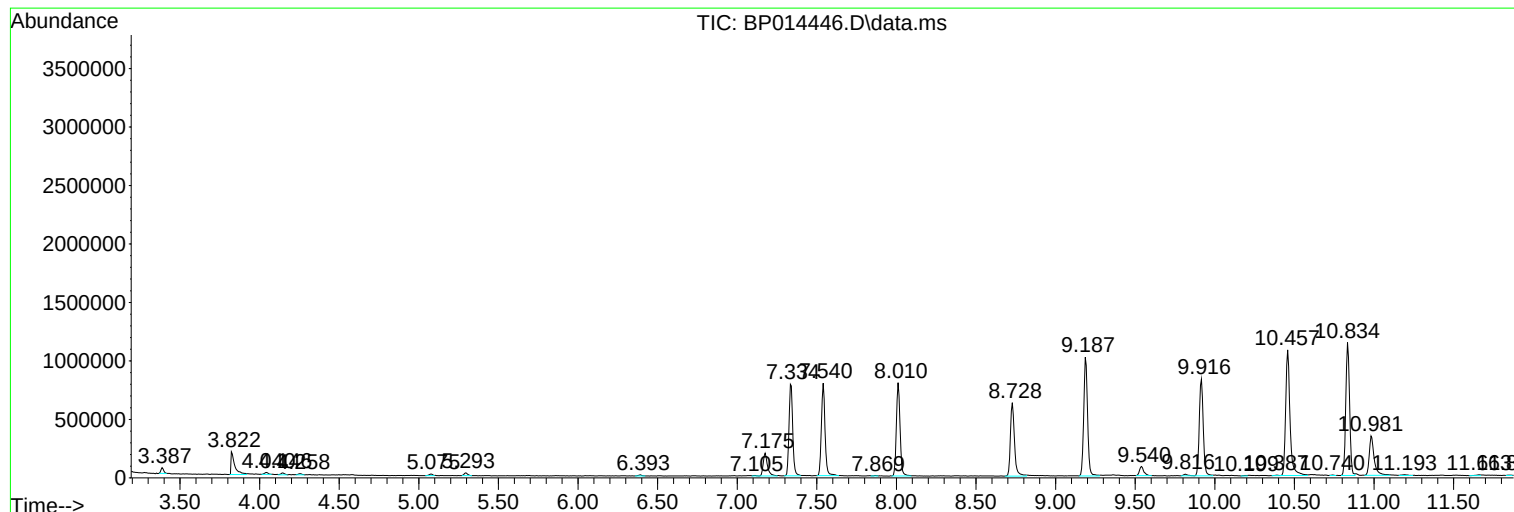
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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014446.D
Acq On : 31 Mar 2023 16:33
Operator : CG/JU
Sample : 02092-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

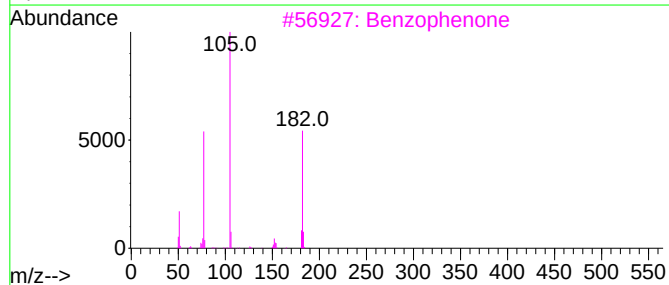
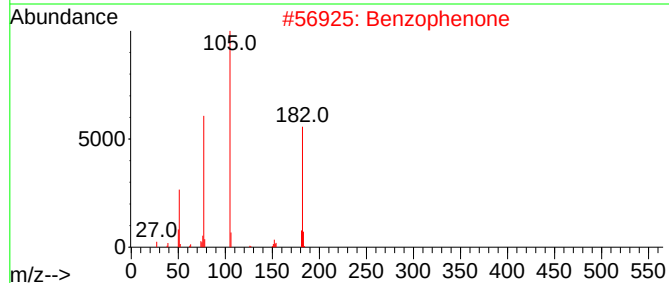
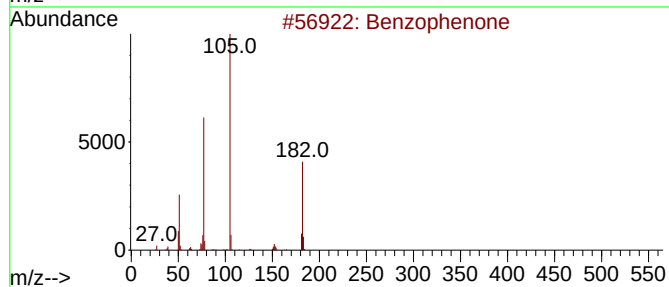
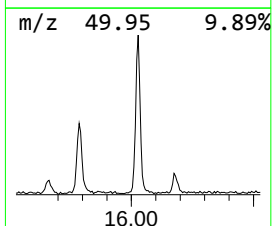
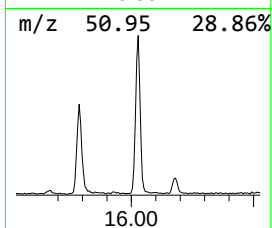
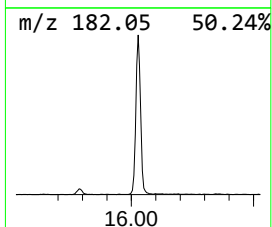
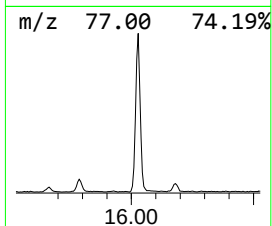
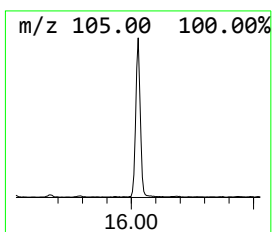
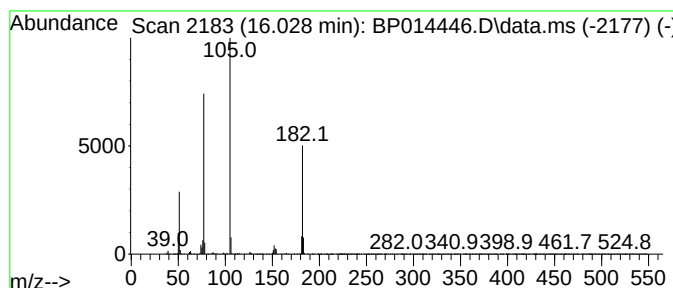
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.028	6.21 ng/ul	726045	Acenaphthene-d10	14.663

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



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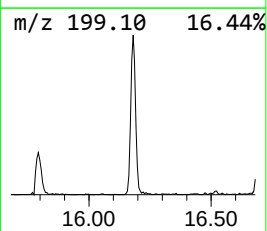
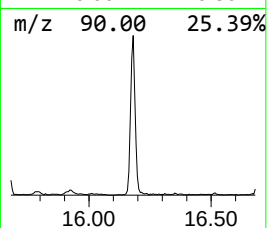
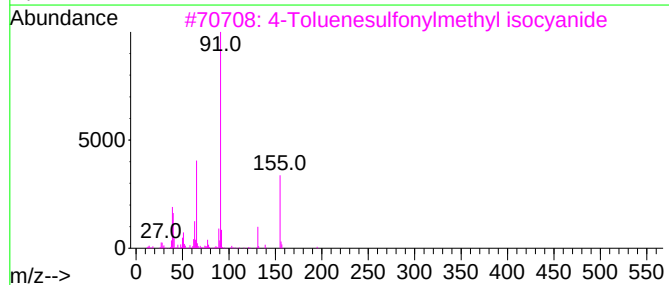
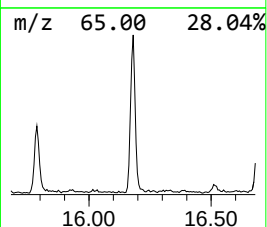
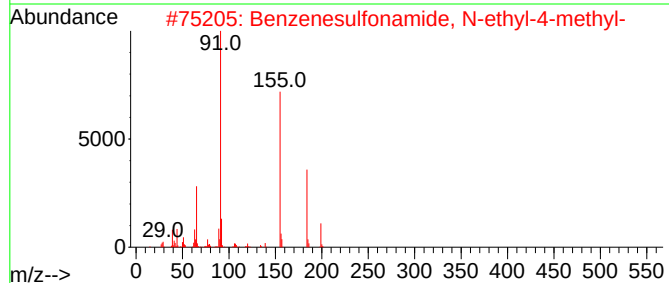
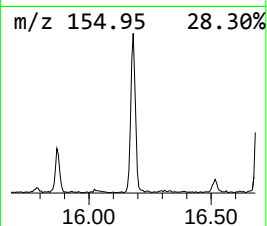
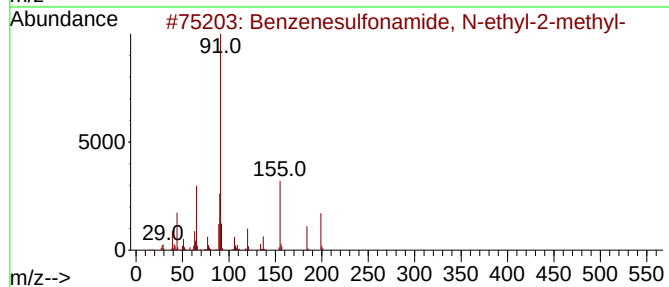
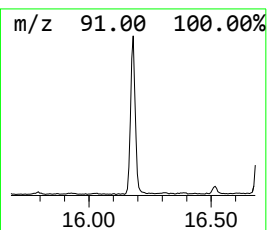
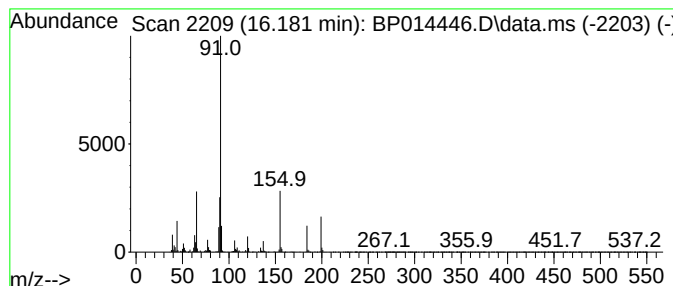
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzenesulfonamide, N-ethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.181	4.48 ng/ul	533451	Phenanthrene-d10	17.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-ethyl-2-me...	199	C9H13NO2S	001077-56-1	98
2			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	59
3			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	52
4			Tolbutamide	270	C12H18N2O3S	000064-77-7	50
5			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50



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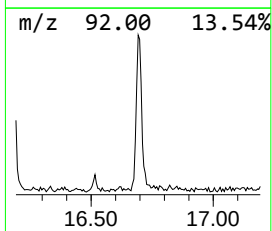
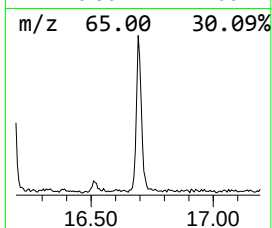
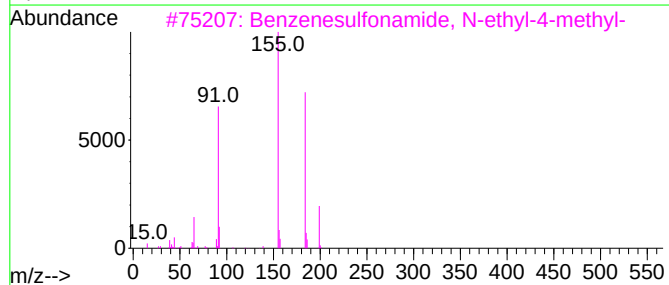
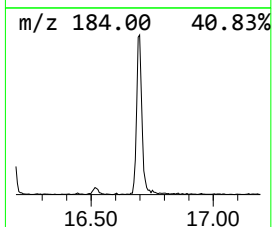
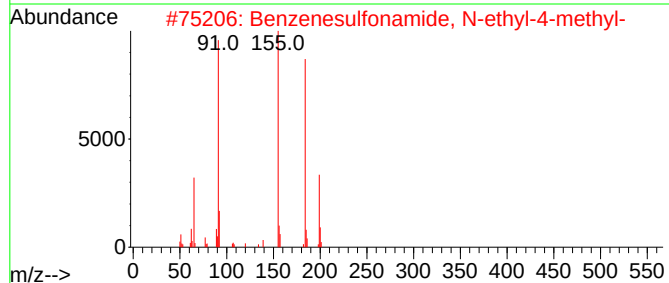
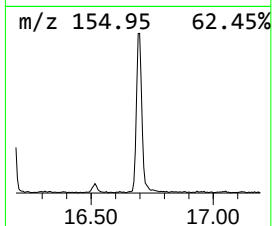
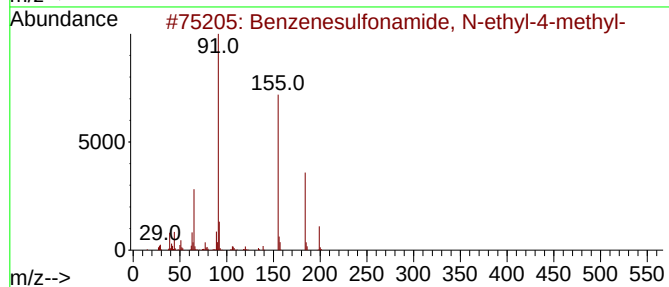
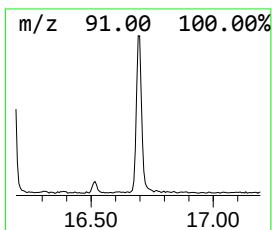
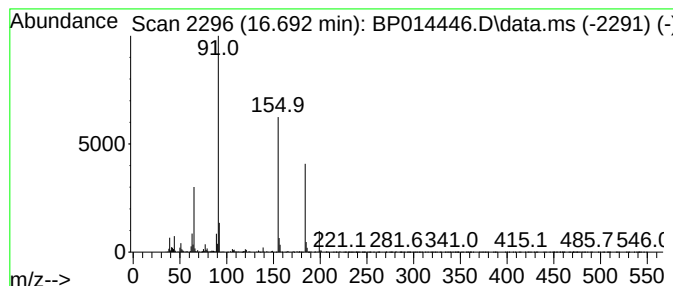
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzenesulfonamide, N-ethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.692	3.50 ng/ul	417119	Phenanthrene-d10	17.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	94
2			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	94
3			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	91
4			N-isobutyl-4-methylbenzenesulfon...	227	C11H17NO2S	023705-38-6	86
5			Benzene, 4-(ethylsulfonyl)-1-met...	184	C9H12O2S	007569-34-8	80



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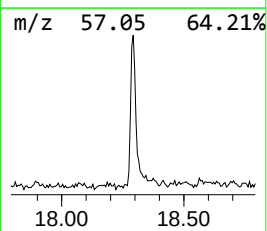
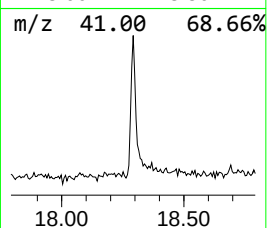
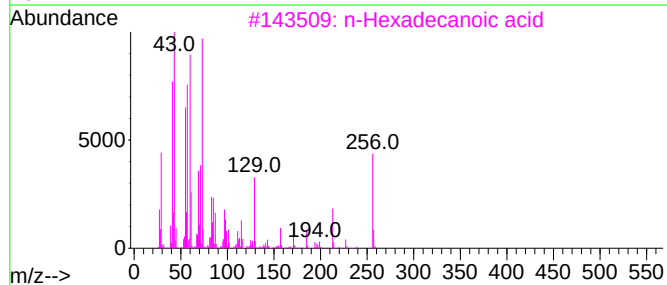
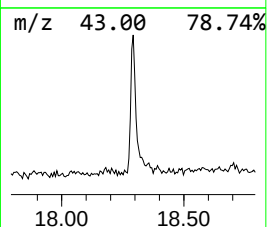
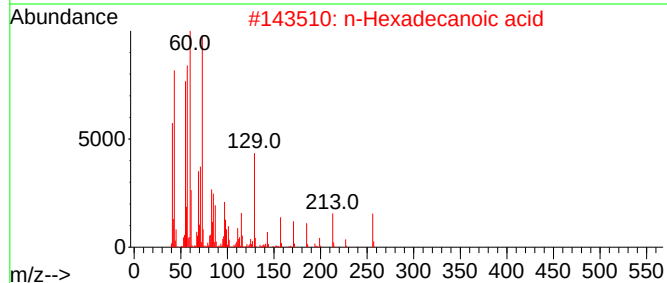
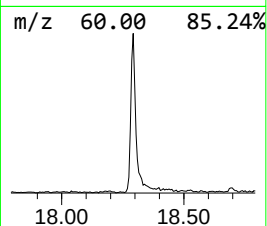
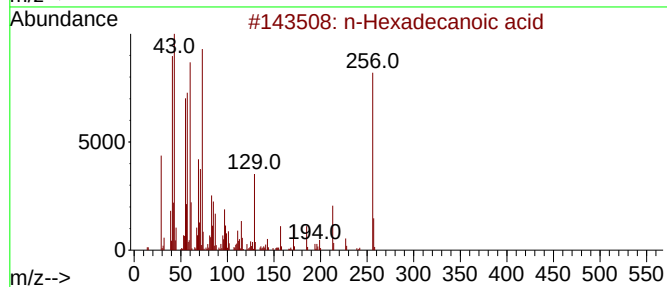
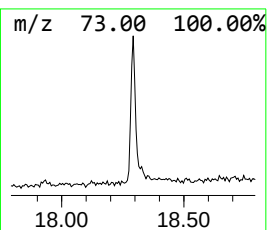
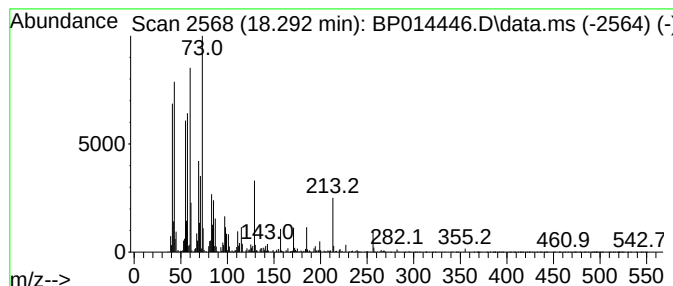
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.292	2.66 ng/ul	317019	Phenanthrene-d10	17.428

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	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014446.D
Acq On : 31 Mar 2023 16:33
Operator : CG/JU
Sample : 02092-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

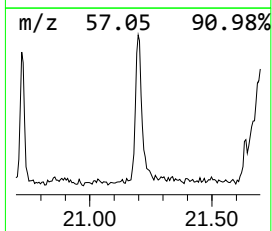
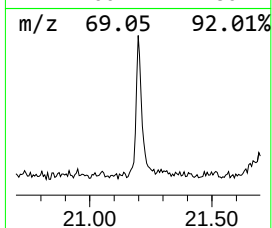
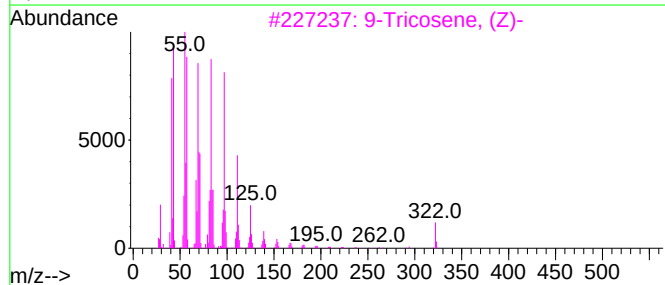
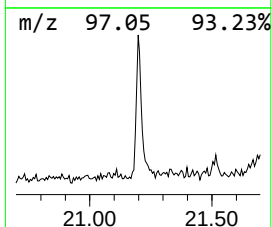
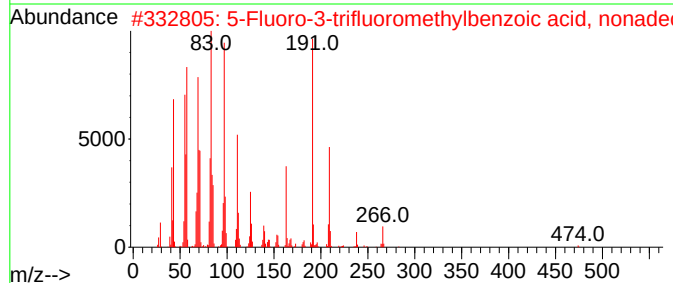
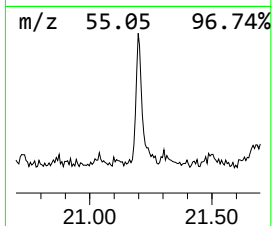
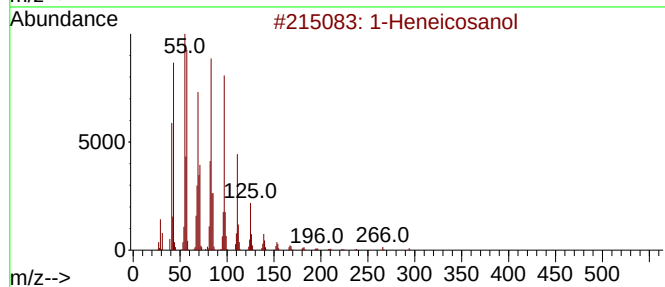
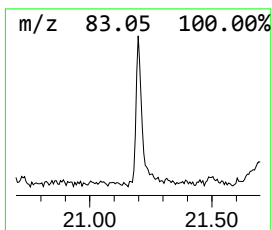
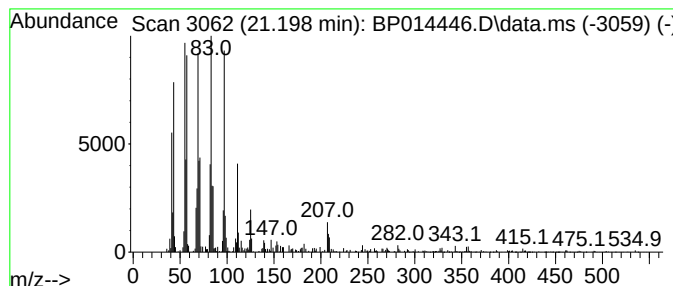
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	2.38 ng/ul	266060	Chrysene-d12	21.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	91
3			9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014446.D
Acq On : 31 Mar 2023 16:33
Operator : CG/JU
Sample : 02092-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

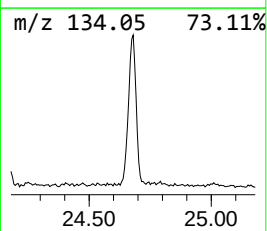
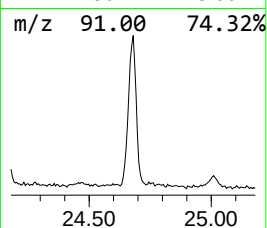
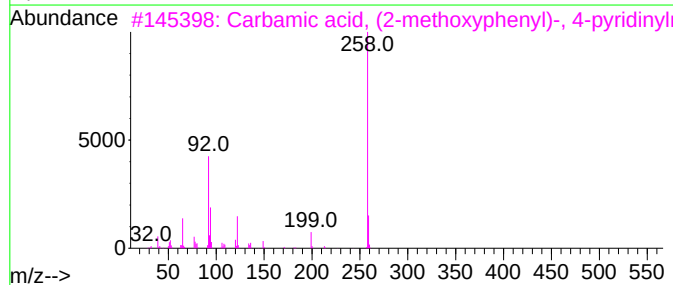
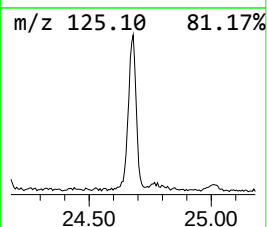
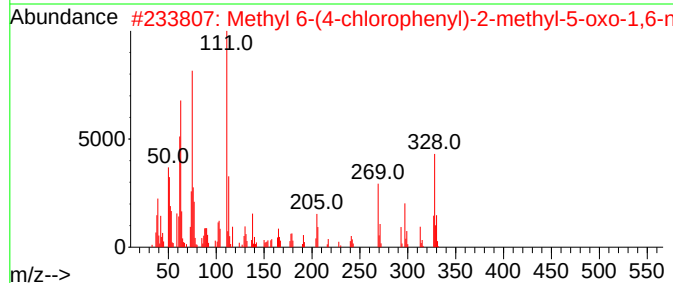
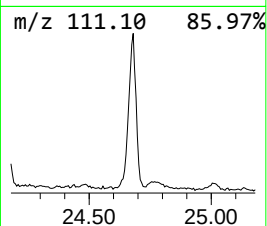
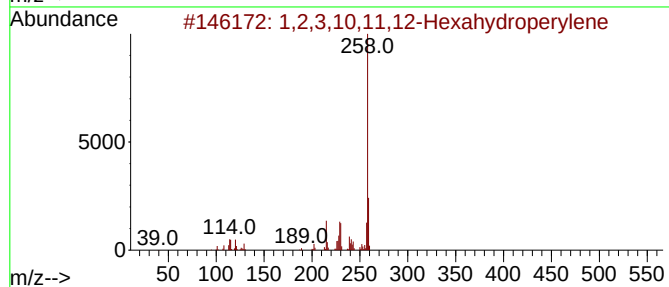
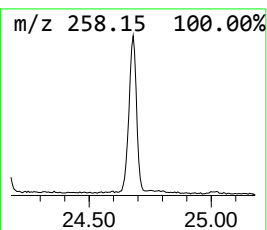
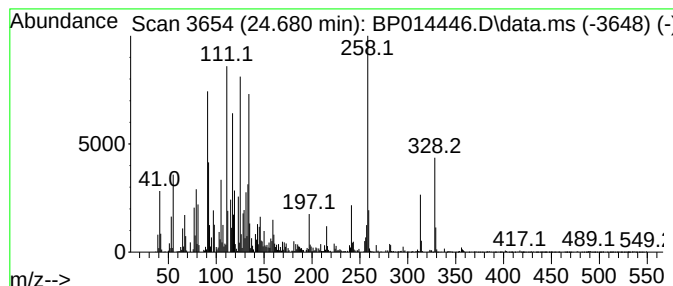
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.680	13.04 ng/ul	1670880	Perylene-d12	24.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,10,11,12-Hexahydroperylene	258	C20H18	007350-92-7	25		
2	Methyl 6-(4-chlorophenyl)-2-meth...	328	C17H13ClN2O3	1000409-65-8	25		
3	Carbamic acid, (2-methoxyphenyl)...	258	C14H14N2O3	1000319-47-1	20		
4	Methanone, (5-methoxy-3-benzofur...	258	C14H10O3S	310456-37-2	18		
5	1,5-Dihydroxy-6-methoxyxanthone	258	C14H10O5	181307-35-7	18		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014446.D
Acq On : 31 Mar 2023 16:33
Operator : CG/JU
Sample : 02092-01
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.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
Benzophenone	16.028	6.2	ng/ul	726045	3	14.663	2337790	20.0
Benzenesulfonam...	16.181	4.5	ng/ul	533451	4	17.428	2382070	20.0
Benzenesulfonam...	16.692	3.5	ng/ul	417119	4	17.428	2382070	20.0
n-Hexadecanoic ...	18.292	2.7	ng/ul	317019	4	17.428	2382070	20.0
1-Heneicosanol	21.198	2.4	ng/ul	266060	5	21.516	2234920	20.0
unknown-01	24.680	13.0	ng/ul	1670880	6	24.033	2561820	20.0