

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
 Data File : BP014447.D
 Acq On : 31 Mar 2023 17:06
 Operator : CG/JU
 Sample : 02093-01
 Misc :
 ALS Vial : 56 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: BP014447.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	30	34	41	rBV	36427	46000	0.80%	0.082%
2	3.822	107	108	129	rBV	163620	310913	5.44%	0.554%
3	4.040	140	145	154	rVB	15481	26142	0.46%	0.047%
4	4.140	159	162	171	rVB	13021	20014	0.35%	0.036%
5	4.252	178	181	186	rVB5	8818	11611	0.20%	0.021%
6	4.581	235	237	247	rVB10	5061	9179	0.16%	0.016%
7	5.075	315	321	326	rBV2	13219	18967	0.33%	0.034%
8	5.293	353	358	364	rVB	20834	34123	0.60%	0.061%
9	6.387	538	544	549	rBV5	7550	12697	0.22%	0.023%
10	7.175	672	678	691	rBV	175146	327435	5.73%	0.583%
11	7.334	697	705	719	rBV	727300	1180463	20.65%	2.103%
12	7.540	734	740	763	rVB	711302	1180572	20.65%	2.103%
13	8.010	812	820	834	rBV	640495	1023075	17.89%	1.823%
14	8.293	865	868	875	rVB9	3049	6404	0.11%	0.011%
15	8.728	932	942	957	rBV	618980	1092359	19.10%	1.946%
16	9.187	1012	1020	1034	rBV	956766	1640070	28.68%	2.922%
17	9.540	1073	1080	1089	rBV2	76064	144138	2.52%	0.257%
18	9.816	1122	1127	1131	rBV6	12592	21276	0.37%	0.038%
19	9.916	1136	1144	1157	rBV	792530	1372744	24.01%	2.446%
20	10.204	1188	1193	1194	rBV5	4086	5796	0.10%	0.010%
21	10.457	1229	1236	1257	rBV	1086181	2060586	36.04%	3.671%
22	10.834	1293	1300	1308	rBV	953671	1573341	27.52%	2.803%
23	10.981	1319	1325	1340	rBV	339650	710737	12.43%	1.266%
24	11.193	1358	1361	1367	rVB8	7261	11901	0.21%	0.021%
25	11.422	1398	1400	1407	rVB8	5245	8575	0.15%	0.015%
26	11.651	1435	1439	1441	rBV5	7552	11264	0.20%	0.020%
27	12.087	1505	1513	1519	rBV5	12164	29715	0.52%	0.053%
28	12.157	1521	1525	1531	rVV9	8877	17132	0.30%	0.031%
29	12.240	1535	1539	1542	rBV5	6100	9712	0.17%	0.017%
30	12.334	1551	1555	1558	rBV6	4232	6941	0.12%	0.012%
31	12.428	1567	1571	1575	rBV3	14061	24241	0.42%	0.043%
32	12.775	1625	1630	1635	rVB9	5670	11823	0.21%	0.021%
33	12.957	1659	1661	1666	rVB4	10305	11216	0.20%	0.020%
34	13.016	1666	1671	1674	rBV7	5659	10359	0.18%	0.018%
35	13.128	1687	1690	1697	rVB7	8895	16026	0.28%	0.029%
36	13.345	1721	1727	1730	rBV7	4930	9962	0.17%	0.018%

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37	13.392	1731	1735	1740	rVV8	5818	11244	0.20%	0.020%
38	13.469	1743	1748	1751	rBV6	12931	18220	0.32%	0.032%
39	13.545	1757	1761	1769	rBV8	9735	20967	0.37%	0.037%
40	13.669	1779	1782	1787	rVB7	11474	16554	0.29%	0.029%
41	13.981	1832	1835	1839	rBV6	5294	9536	0.17%	0.017%
42	14.075	1842	1851	1864	rVV	2545911	3660023	64.01%	6.521%
43	14.175	1866	1868	1871	rVB4	8485	9513	0.17%	0.017%
44	14.257	1879	1882	1885	rBV5	5477	7945	0.14%	0.014%
45	14.304	1887	1890	1893	rVV5	8910	11451	0.20%	0.020%
46	14.363	1893	1900	1913	rVB	2762209	4050846	70.85%	7.217%
47	14.616	1940	1943	1945	rBV	13341	13274	0.23%	0.024%
48	14.669	1945	1952	1958	rVV	1483104	2193771	38.37%	3.908%
49	14.910	1988	1993	2007	rBV	83289	235719	4.12%	0.420%
50	15.481	2087	2090	2094	rBV	22870	30267	0.53%	0.054%
51	15.663	2114	2121	2133	rBV	3684910	5117221	89.50%	9.117%
52	15.786	2136	2142	2150	rBV	1242674	1816569	31.77%	3.236%
53	15.869	2152	2156	2160	rBV	129344	151011	2.64%	0.269%
54	16.028	2178	2183	2190	rBV	650537	856749	14.98%	1.526%
55	16.181	2204	2209	2215	rBV	492646	667054	11.67%	1.188%
56	16.516	2263	2266	2270	rBV	21621	24311	0.43%	0.043%
57	16.598	2276	2280	2286	rBV6	17179	37146	0.65%	0.066%
58	16.698	2292	2297	2301	rBV	343608	494863	8.65%	0.882%
59	17.428	2415	2421	2430	rBV	1862349	2564896	44.86%	4.570%
60	17.528	2432	2438	2446	rVV2	3612659	5255449	91.92%	9.363%
61	18.292	2564	2568	2577	rBV	313941	455112	7.96%	0.811%
62	18.704	2635	2638	2647	rVB	51419	68276	1.19%	0.122%
63	19.333	2742	2745	2750	rBV2	47314	58301	1.02%	0.104%
64	19.522	2773	2777	2782	rBV2	133047	200866	3.51%	0.358%
65	19.757	2811	2817	2822	rBV	4359477	5717670	100.00%	10.186%
66	20.727	2979	2982	2986	rVB3	97231	108132	1.89%	0.193%
67	21.198	3059	3062	3068	rBV2	195227	280614	4.91%	0.500%
68	21.516	3111	3116	3123	rBV	1405687	1906941	33.35%	3.397%
69	23.868	3509	3516	3528	rBV2	1961471	3941930	68.94%	7.023%
70	24.033	3538	3544	3558	rVB2	823061	1770917	30.97%	3.155%
71	24.674	3648	3653	3663	rVB3	595554	1339026	23.42%	2.386%

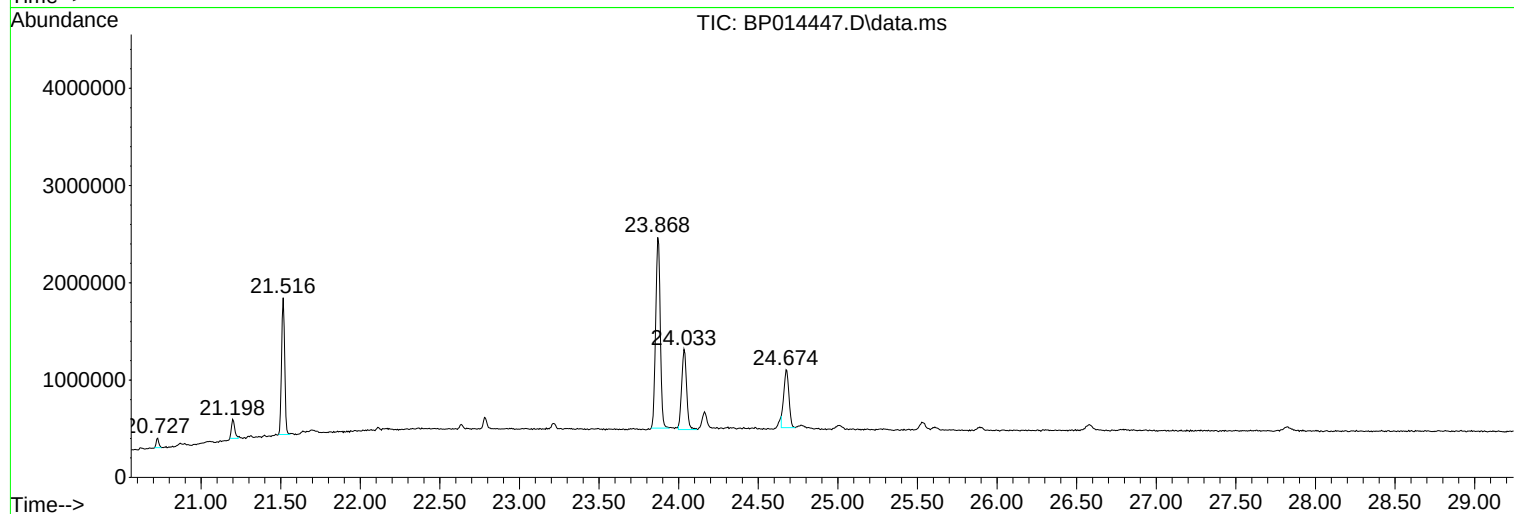
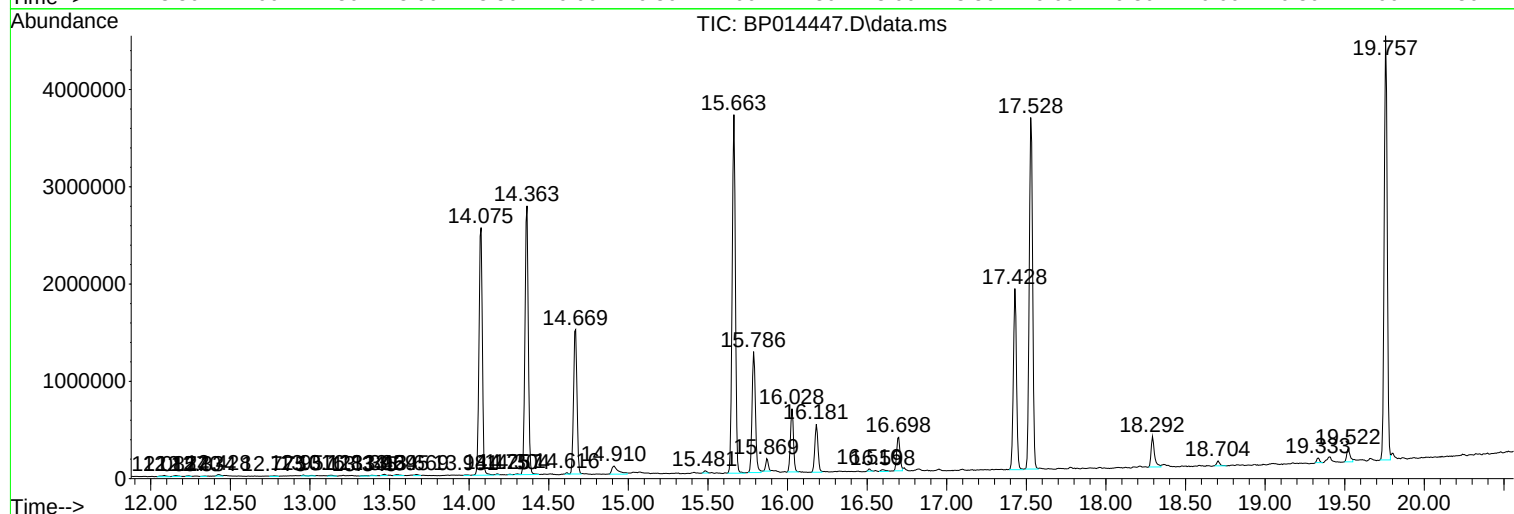
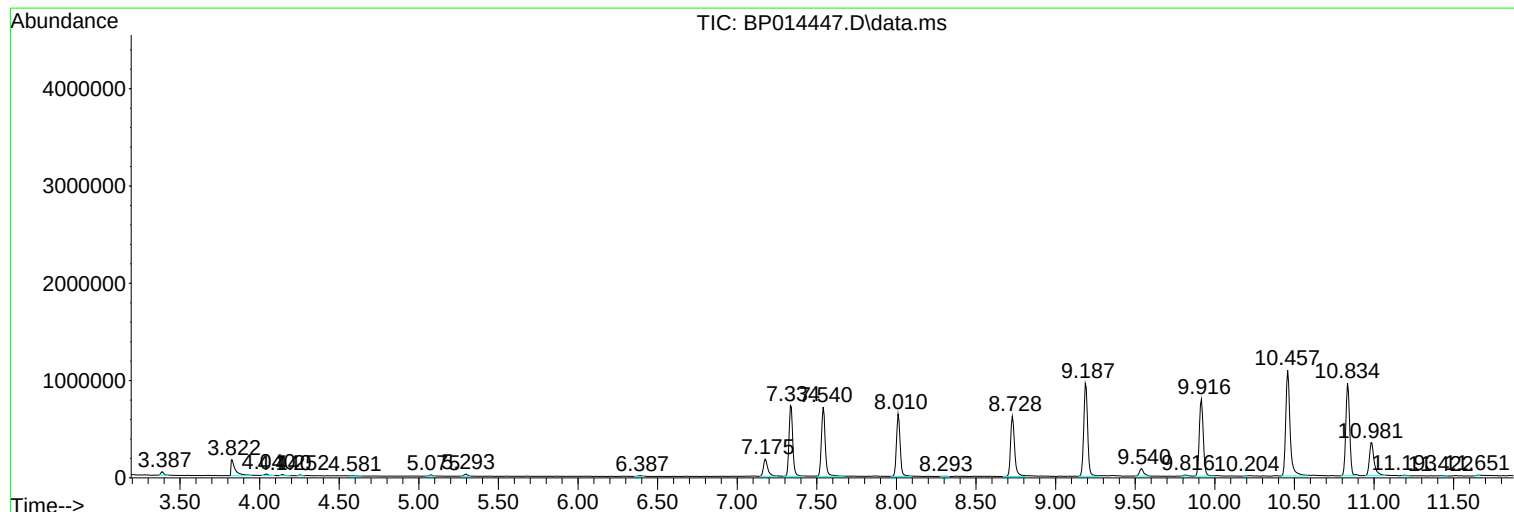
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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



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Data File : BP014447.D
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Operator : CG/JU
Sample : 02093-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

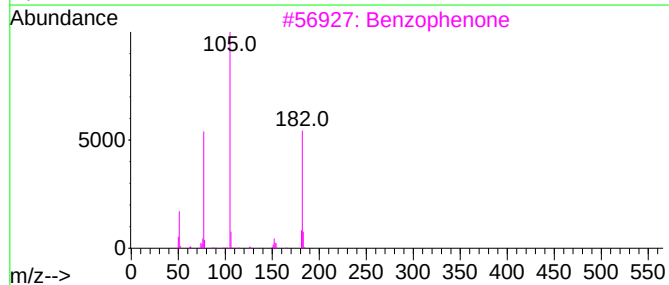
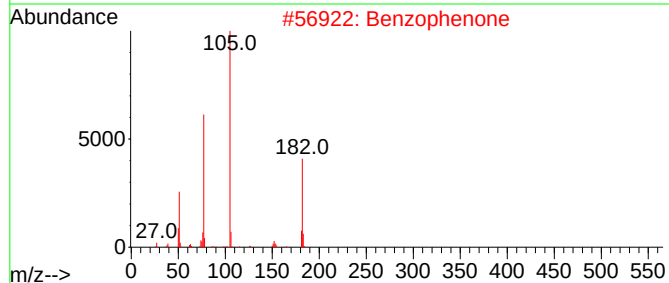
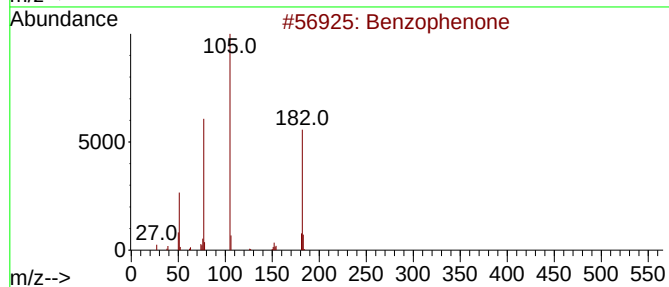
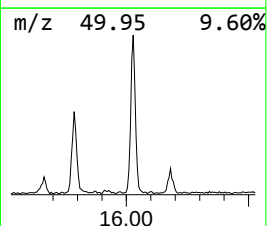
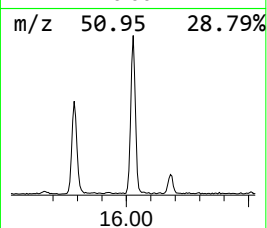
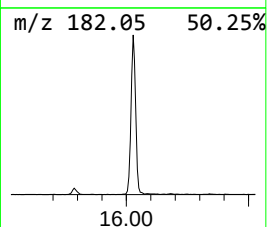
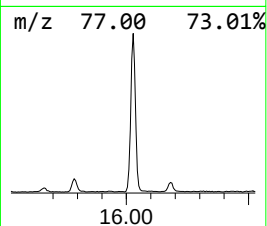
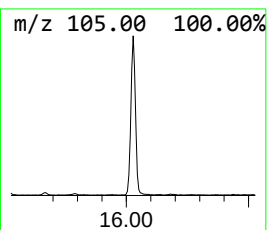
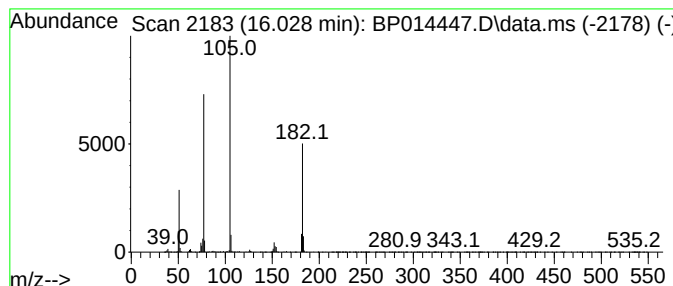
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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	7.81 ng/ul	856749	Acenaphthene-d10	14.669

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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ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

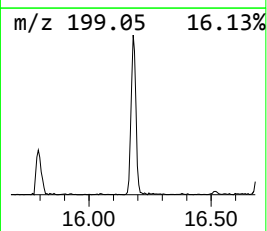
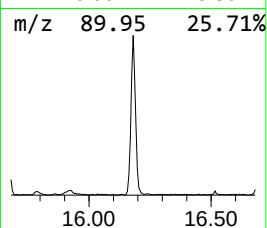
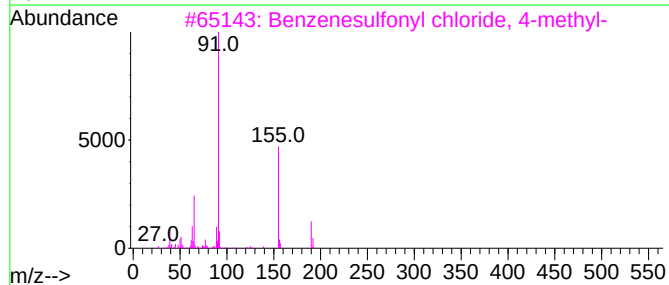
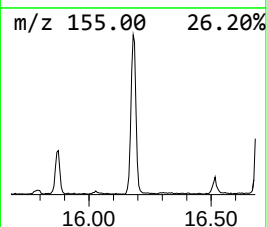
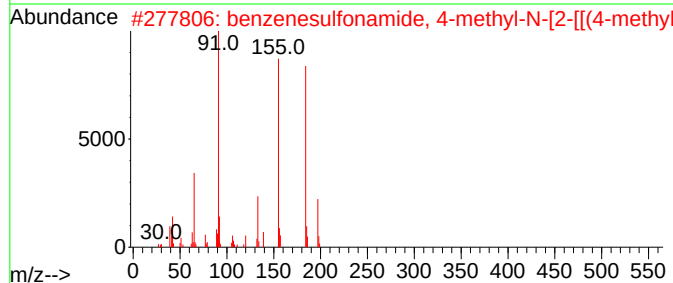
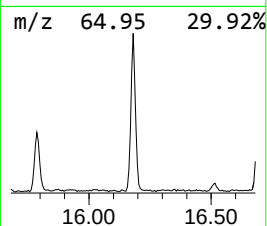
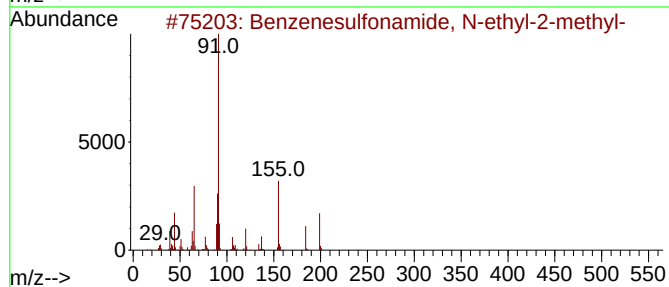
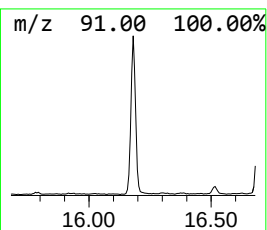
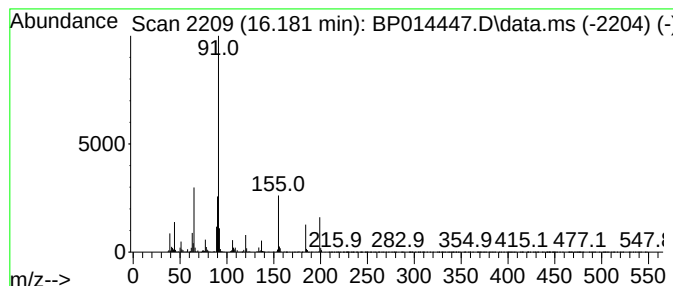
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.180	5.20 ng/ul	667054	Phenanthrene-d10	17.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-ethyl-2-me...	199	C9H13NO2S	001077-56-1	98
2			benzenesulfonamide, 4-methyl-N-[...	369	C16H19NO5S2	1000402-61-7	59
3			Benzenesulfonyl chloride, 4-methyl-	190	C7H7ClO2S	000098-59-9	50
4			Tolbutamide	270	C12H18N2O3S	000064-77-7	50
5			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	49



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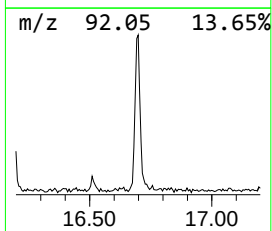
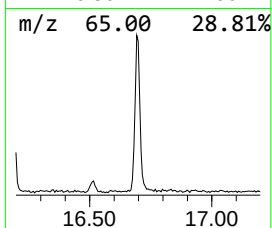
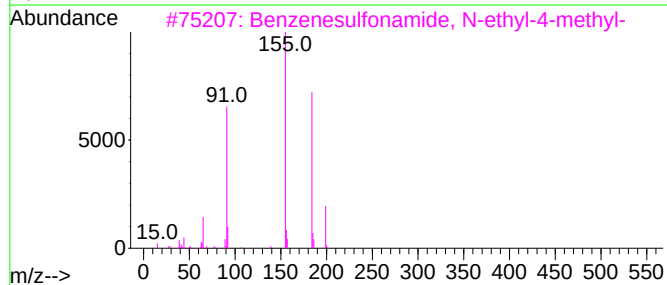
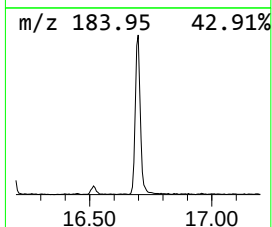
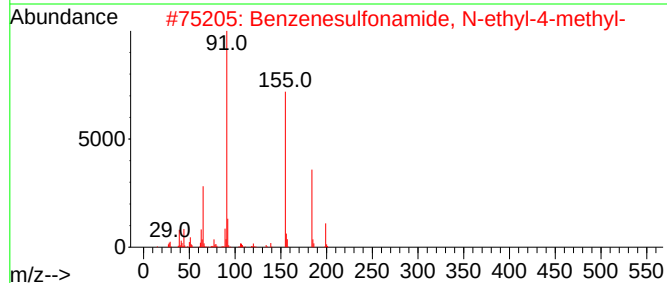
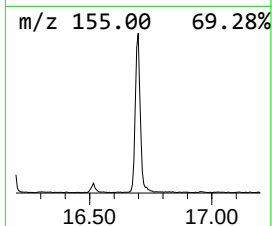
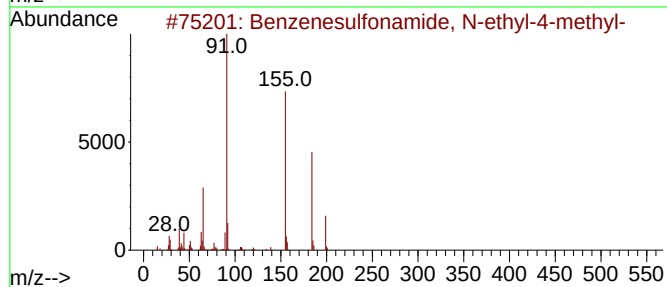
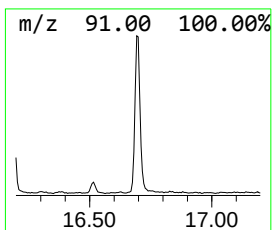
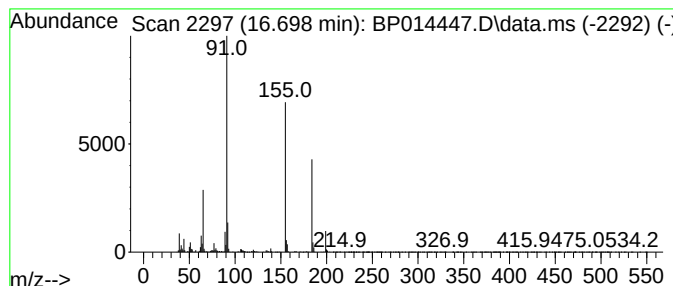
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Quant Title : SVOA CALIBRATION

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.
16.698	3.86 ng/ul	494863	Phenanthrene-d10	17.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	97
2			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	96
3			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	94
4			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	91
5			4-Methyl-N-(2-oxobutyl)benzenesu...	241	C11H15NO3S	1000192-14-5	86



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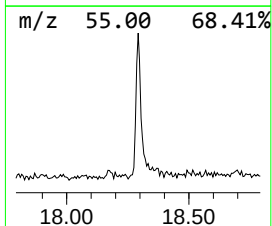
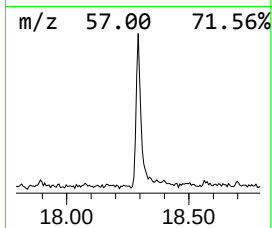
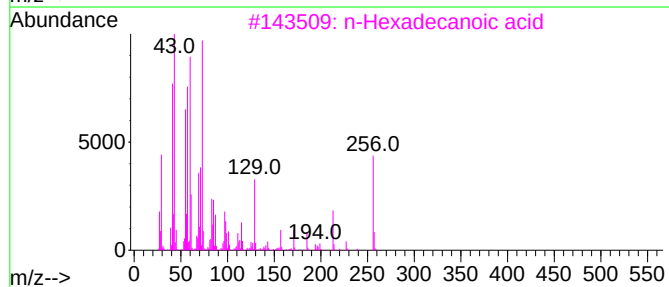
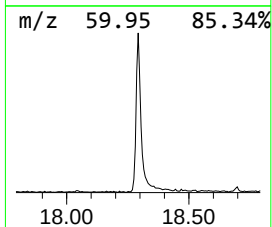
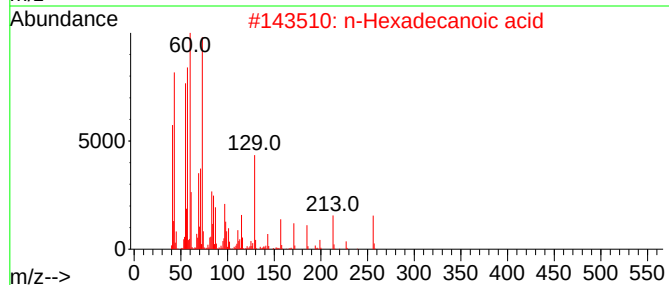
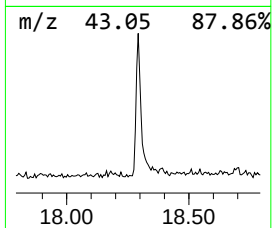
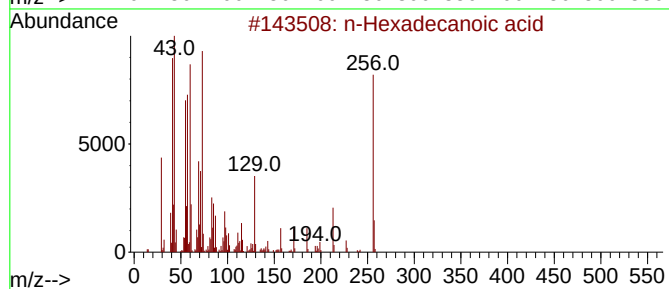
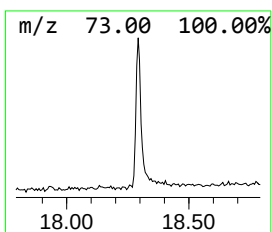
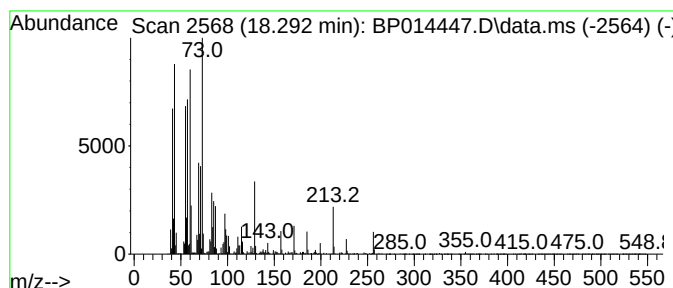
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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	3.55 ng/ul	455112	Phenanthrene-d10	17.427

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	98
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014447.D
Acq On : 31 Mar 2023 17:06
Operator : CG/JU
Sample : 02093-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

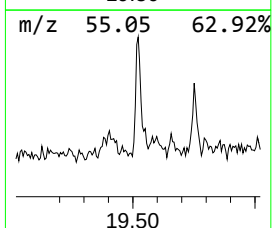
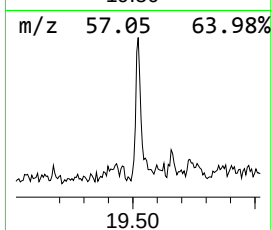
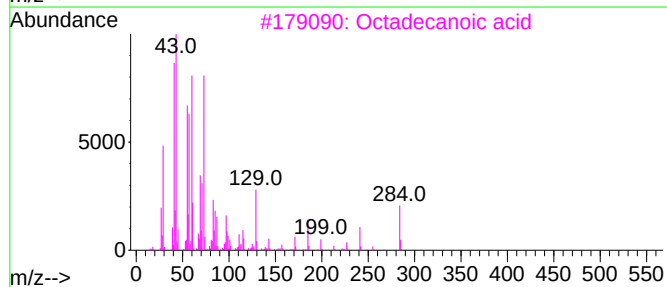
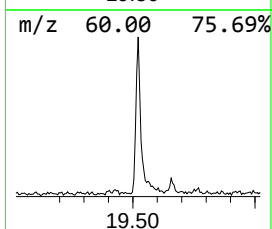
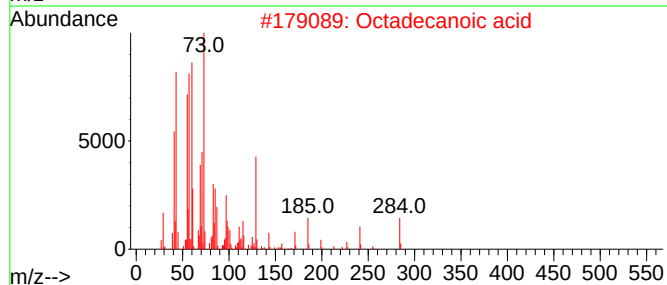
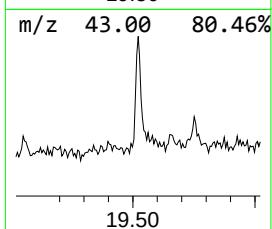
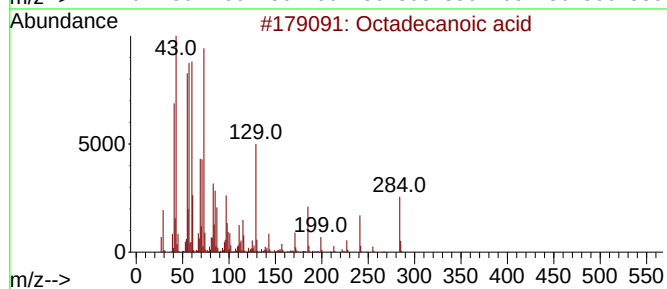
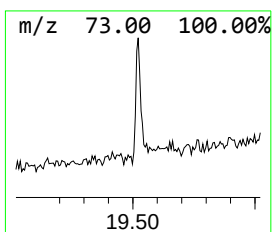
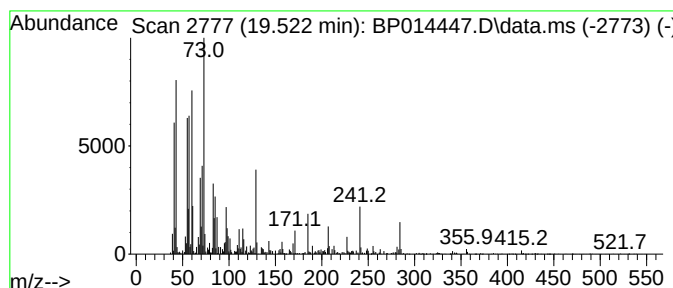
Instrument :
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ClientSampleId :
CB964

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 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.522	2.11 ng/ul	200866	Chrysene-d12		21.516	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	98
2	Octadecanoic acid		284	C18H36O2	000057-11-4	95
3	Octadecanoic acid		284	C18H36O2	000057-11-4	94
4	Octadecanoic acid		284	C18H36O2	000057-11-4	94
5	Octadecanoic acid		284	C18H36O2	000057-11-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014447.D
Acq On : 31 Mar 2023 17:06
Operator : CG/JU
Sample : 02093-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

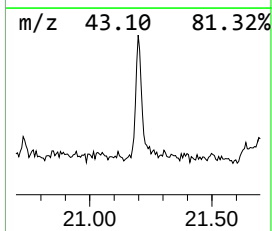
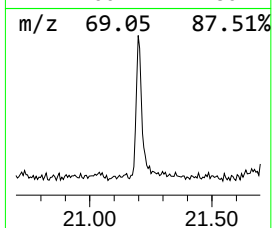
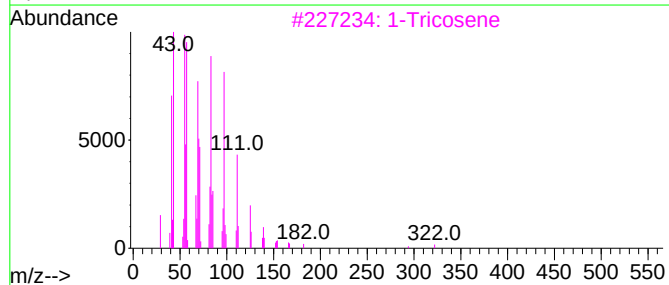
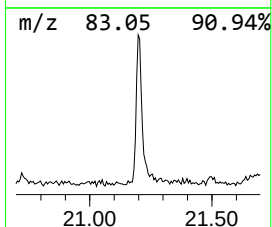
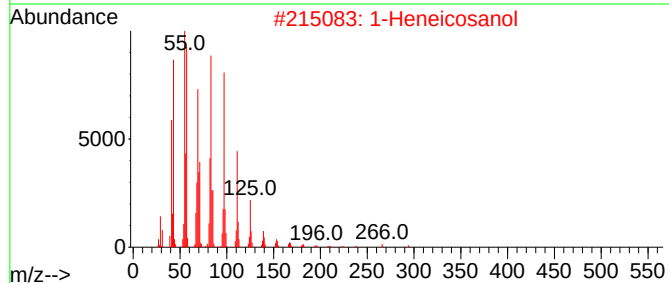
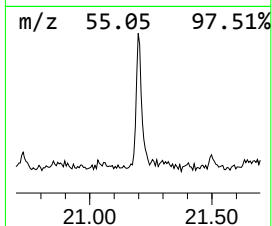
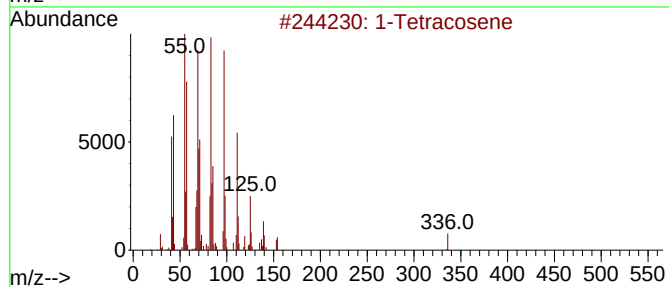
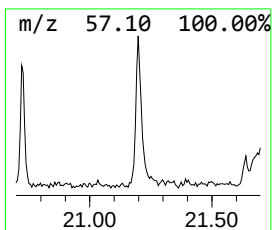
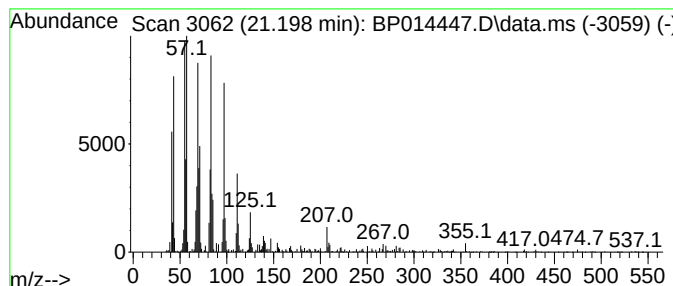
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.198	2.94 ng/ul	280614	Chrysene-d12	21.516	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Tricosene	322	C23H46	018835-32-0	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Octadecanol	270	C18H38O	000112-92-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014447.D
Acq On : 31 Mar 2023 17:06
Operator : CG/JU
Sample : 02093-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB964

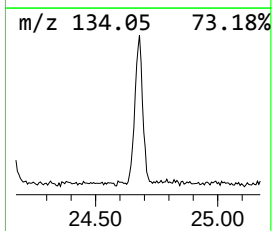
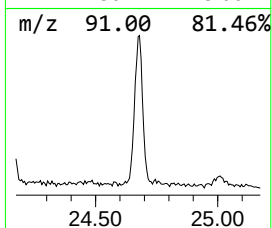
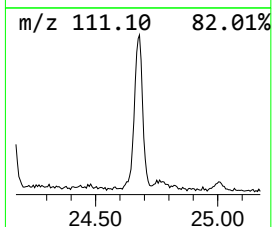
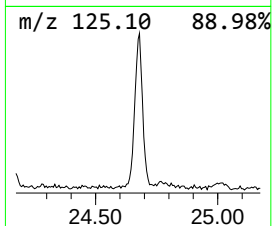
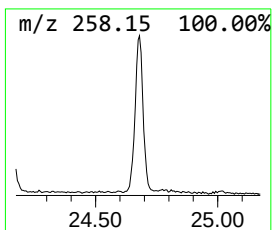
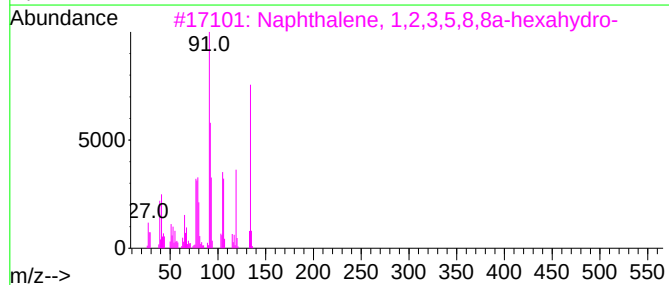
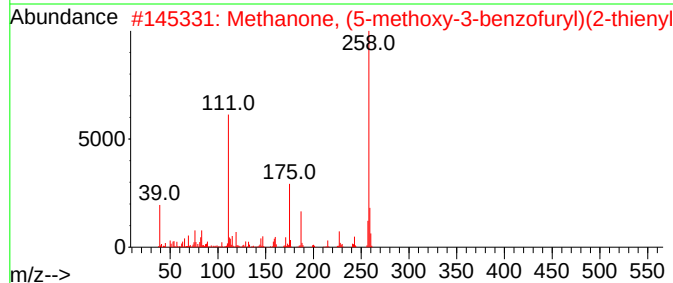
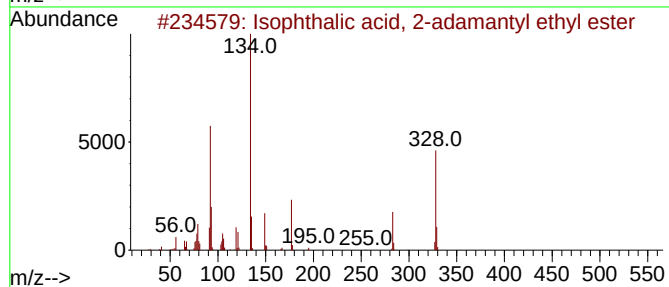
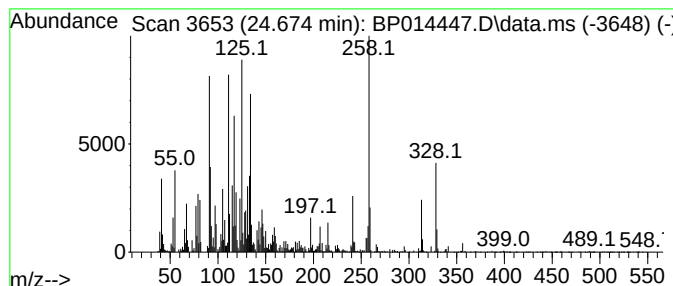
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP032823.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 Isophthalic acid, 2-adamant... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.674	15.12 ng/ul	1339030	Perylene-d12	24.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isophthalic acid, 2-adamantyl et...	328	C20H24O4	1000343-95-9	51
2			Methanone, (5-methoxy-3-benzofur...	258	C14H10O3S	310456-37-2	30
3			Naphthalene, 1,2,3,5,8,8a-hexahy...	134	C10H14	062690-65-7	25
4			Carbamic acid, (2-methoxyphenyl)...	258	C14H14N2O3	1000319-47-1	18
5			1-(4-Ethyl-phenyl)-5-oxo-pyrroli...	328	C20H28N2O2	1010275-50-2	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033023\
Data File : BP014447.D
Acq On : 31 Mar 2023 17:06
Operator : CG/JU
Sample : 02093-01
Misc :
ALS Vial : 56 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	7.8	ng/ul	856749	3	14.669	2193770	20.0
Benzenesulfonam...	16.180	5.2	ng/ul	667054	4	17.427	2564900	20.0
Benzenesulfonam...	16.698	3.9	ng/ul	494863	4	17.427	2564900	20.0
n-Hexadecanoic ...	18.292	3.5	ng/ul	455112	4	17.427	2564900	20.0
Octadecanoic acid	19.522	2.1	ng/ul	200866	5	21.516	1906940	20.0
(DEL) Alkane: S...	21.198	2.9	ng/ul	280614	5	21.516	1906940	20.0
Isophthalic aci...	24.674	15.1	ng/ul	1339030	6	24.033	1770920	20.0