

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061424\
 Data File : BM046037.D
 Acq On : 14 Jun 2024 13:43
 Operator : MA/JU
 Sample : P2695-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A4BJ9

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_M\Methods\SFAM-EPA-BM053124.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM046037.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	6	9	19	rVB2	29655	51277	2.04%	0.148%
2	3.499	83	87	89	rBV4	20028	32788	1.30%	0.095%
3	3.528	89	92	100	rVB2	33980	54622	2.17%	0.158%
4	3.693	116	120	122	rBV5	7197	11268	0.45%	0.033%
5	3.722	123	125	129	rVB4	12892	10727	0.43%	0.031%
6	3.893	152	154	159	rVB6	5229	8731	0.35%	0.025%
7	4.104	187	190	193	rVV4	4263	4322	0.17%	0.012%
8	4.140	193	196	202	rVB4	10373	15621	0.62%	0.045%
9	4.216	205	209	212	rBV	15725	22739	0.90%	0.066%
10	4.263	213	217	223	rVB	33463	46735	1.86%	0.135%
11	4.481	248	254	260	rVB9	7321	16407	0.65%	0.047%
12	4.622	271	278	293	rVV	67995	136531	5.43%	0.395%
13	6.034	515	518	521	rVB5	2996	3121	0.12%	0.009%
14	6.110	530	531	535	rVB4	2755	3155	0.13%	0.009%
15	6.369	569	575	579	rBV9	1895	4054	0.16%	0.012%
16	6.622	615	618	620	rVV3	3000	3955	0.16%	0.011%
17	6.692	623	630	642	rVV	500941	997991	39.67%	2.885%
18	6.798	643	648	669	rVB	361458	692415	27.52%	2.002%
19	6.992	675	681	692	rBV	552190	959000	38.12%	2.772%
20	7.257	722	726	729	rBV5	2684	4541	0.18%	0.013%
21	7.334	734	739	741	rVV6	3000	4158	0.17%	0.012%
22	7.434	749	756	769	rBV	522568	857717	34.09%	2.480%
23	7.557	775	777	783	rVB7	2548	2873	0.11%	0.008%
24	7.969	846	847	850	rBV3	2949	3199	0.13%	0.009%
25	8.204	880	887	897	rBV	520949	1009977	40.14%	2.920%
26	8.286	897	901	917	rVB3	36240	96588	3.84%	0.279%
27	8.598	947	954	966	rBV	563981	986406	39.21%	2.852%
28	8.875	998	1001	1004	rVB4	3296	3782	0.15%	0.011%
29	8.992	1019	1021	1024	rVB4	4088	3324	0.13%	0.010%
30	9.039	1026	1029	1032	rBV4	2082	3118	0.12%	0.009%
31	9.204	1053	1057	1060	rBV5	2513	4364	0.17%	0.013%
32	9.310	1068	1075	1091	rBV	470430	865886	34.42%	2.503%
33	9.639	1127	1131	1134	rBV5	4579	6525	0.26%	0.019%
34	9.704	1137	1142	1146	rVV7	4876	11266	0.45%	0.033%
35	9.863	1162	1169	1194	rBV	491440	1134407	45.09%	3.280%
36	10.198	1219	1226	1241	rBV	665727	1186591	47.16%	3.430%

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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_M\Methods\SFAM-EPA-BM053124.MA.M
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37	10.392	1251	1259	1279	rBV	334836	871454	34.64%	2.519%
38	11.039	1361	1369	1379	rBV6	11343	34441	1.37%	0.100%
39	11.122	1380	1383	1385	rVV4	4429	6103	0.24%	0.018%
40	11.145	1385	1387	1392	rVB5	4205	6457	0.26%	0.019%
41	11.263	1404	1407	1409	rVB3	3120	2943	0.12%	0.009%
42	11.816	1495	1501	1509	rVB7	8659	21012	0.84%	0.061%
43	11.892	1512	1514	1516	rBV3	3397	3099	0.12%	0.009%
44	12.127	1549	1554	1557	rBV6	2353	3949	0.16%	0.011%
45	12.274	1574	1579	1583	rBV6	2297	4020	0.16%	0.012%
46	12.469	1608	1612	1615	rVV5	3077	3965	0.16%	0.011%
47	13.033	1703	1708	1716	rBV2	20343	43550	1.73%	0.126%
48	13.527	1786	1792	1807	rBV	920725	1524309	60.58%	4.407%
49	13.668	1815	1816	1820	rVB4	3284	3230	0.13%	0.009%
50	13.768	1826	1833	1849	rBV	1158209	1785109	70.95%	5.161%
51	14.010	1870	1874	1877	rVB5	2720	3243	0.13%	0.009%
52	14.080	1879	1886	1894	rVV	928829	1430198	56.84%	4.135%
53	14.139	1894	1896	1902	rVB4	7873	12974	0.52%	0.038%
54	14.339	1921	1930	1934	rBV	770608	1790735	71.17%	5.177%
55	14.386	1934	1938	1958	rVB	385196	915273	36.38%	2.646%
56	14.810	2009	2010	2015	rBV5	2585	3094	0.12%	0.009%
57	14.951	2030	2034	2037	rVB6	5330	8263	0.33%	0.024%
58	15.080	2049	2056	2064	rBV	1411260	2091920	83.14%	6.048%
59	15.162	2068	2070	2075	rVV4	13924	19045	0.76%	0.055%
60	15.227	2075	2081	2093	rVV	431224	664692	26.42%	1.922%
61	15.321	2095	2097	2101	rVB5	7597	8888	0.35%	0.026%
62	15.821	2180	2182	2186	rVV5	5795	6755	0.27%	0.020%
63	15.862	2188	2189	2194	rVV5	5481	6176	0.25%	0.018%
64	16.298	2258	2263	2267	rBV8	7137	11851	0.47%	0.034%
65	16.333	2267	2269	2272	rVB4	2965	2920	0.12%	0.008%
66	16.404	2277	2281	2286	rVV7	8140	14642	0.58%	0.042%
67	16.504	2296	2298	2304	rVB7	6591	9196	0.37%	0.027%
68	16.556	2304	2307	2309	rBV4	3962	4949	0.20%	0.014%
69	16.615	2313	2317	2318	rBV4	7340	8895	0.35%	0.026%
70	16.774	2342	2344	2347	rBV4	3705	4635	0.18%	0.013%
71	16.827	2347	2353	2357	rVV	1145775	1616223	64.24%	4.672%
72	16.862	2357	2359	2364	rVV	105228	141697	5.63%	0.410%
73	16.927	2364	2370	2385	rVB	1493484	2201921	87.52%	6.366%
74	17.045	2386	2390	2393	rBV5	4693	8119	0.32%	0.023%
75	17.262	2417	2427	2430	rBV7	11848	29071	1.16%	0.084%
76	17.439	2450	2457	2465	rBV7	8355	17982	0.71%	0.052%

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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

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77	17.521	2467	2471	2474	rBV4	16177	19743	0.78%	0.057%
78	17.633	2487	2490	2498	rVB9	5985	11597	0.46%	0.034%
79	17.703	2498	2502	2506	rBV6	13056	22468	0.89%	0.065%
80	17.756	2506	2511	2520	rBV	228061	427610	17.00%	1.236%
81	17.903	2531	2536	2539	rBV3	27088	37790	1.50%	0.109%
82	18.015	2551	2555	2559	rVB7	8843	16547	0.66%	0.048%
83	18.068	2561	2564	2570	rVB4	12998	17726	0.70%	0.051%
84	18.215	2583	2589	2592	rBV7	11665	25636	1.02%	0.074%
85	18.374	2612	2616	2619	rVB6	10366	14519	0.58%	0.042%
86	18.674	2663	2667	2669	rBV4	21999	30482	1.21%	0.088%
87	18.698	2669	2671	2674	rVB2	37619	39802	1.58%	0.115%
88	18.768	2680	2683	2685	rBV4	25058	34948	1.39%	0.101%
89	18.845	2691	2696	2697	rBV4	23619	35169	1.40%	0.102%
90	18.892	2700	2704	2709	rVB	206198	263398	10.47%	0.761%
91	19.045	2726	2730	2737	rBV2	106588	196488	7.81%	0.568%
92	19.227	2755	2761	2770	rBV	1800612	2515994	100.00%	7.274%
93	20.286	2939	2941	2945	rVB3	33030	37923	1.51%	0.110%
94	20.750	3017	3020	3027	rBV	160547	242164	9.62%	0.700%
95	20.974	3055	3058	3062	rBV	82751	96780	3.85%	0.280%
96	21.039	3063	3069	3074	rBV	1281705	1851890	73.60%	5.354%
97	21.733	3184	3187	3190	rBV3	91649	118293	4.70%	0.342%
98	22.956	3392	3395	3402	rVB	181597	289124	11.49%	0.836%
99	23.562	3491	3498	3505	rBV2	877308	1726911	68.64%	4.992%
100	23.744	3522	3529	3537	rVB	840205	1910131	75.92%	5.522%

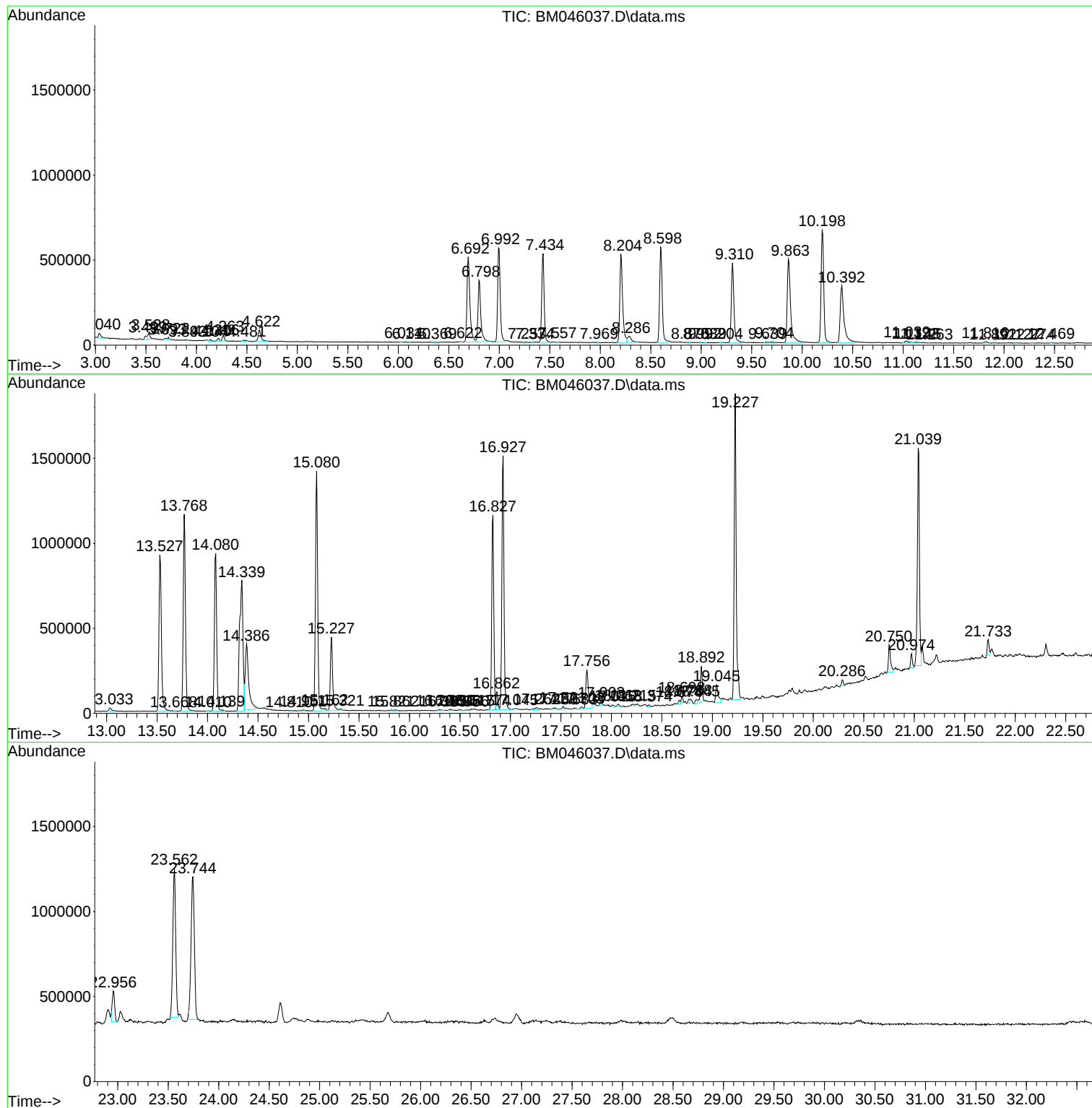
Sum of corrected areas: 34590312

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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



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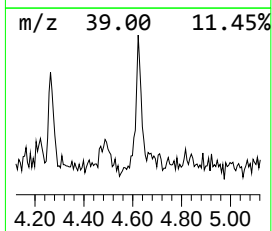
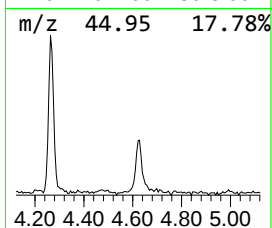
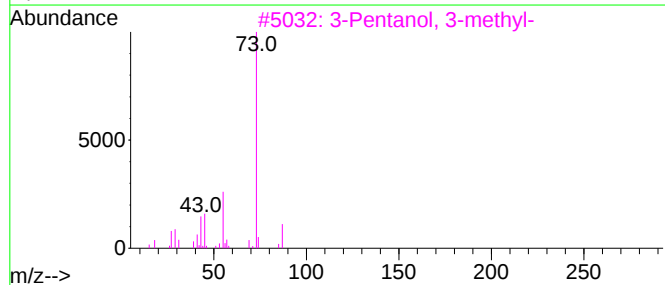
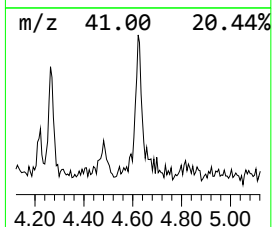
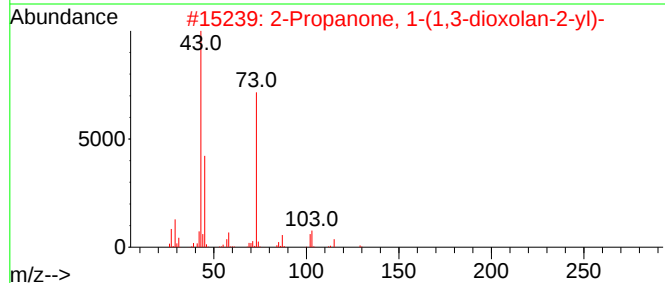
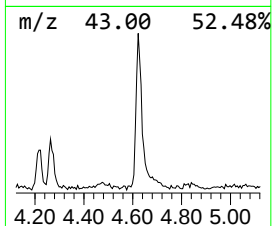
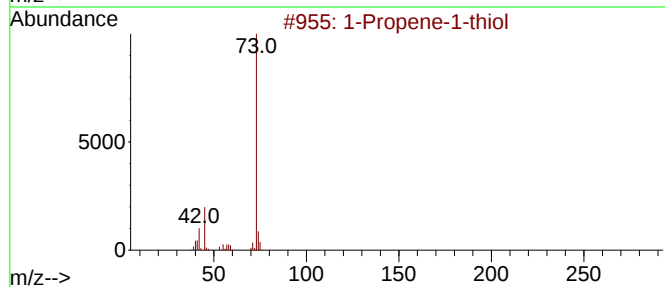
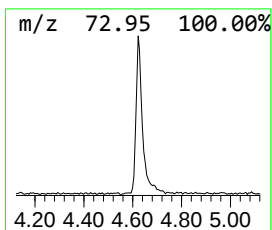
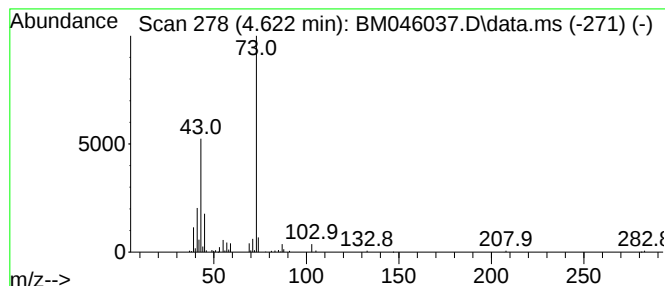
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.622	3.18 ng/ul	136531	1,4-Dichlorobenzene-d4	7.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propene-1-thiol	74	C3H6S	000925-89-3	47
2			2-Propanone, 1-(1,3-dioxolan-2-yl)-	130	C6H10O3	000767-04-4	38
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	38



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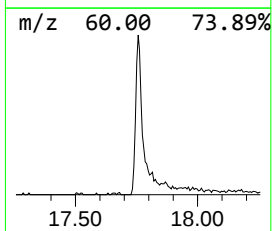
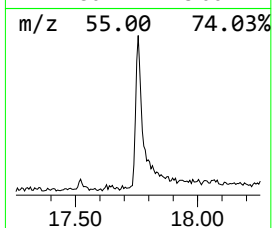
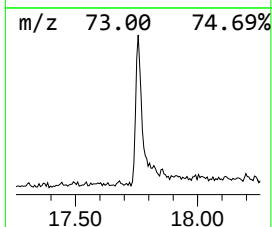
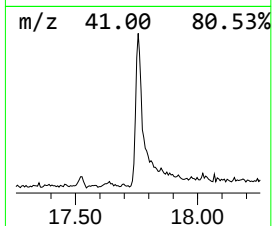
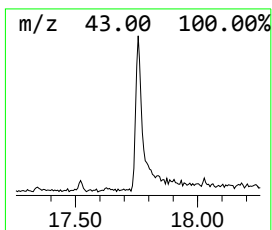
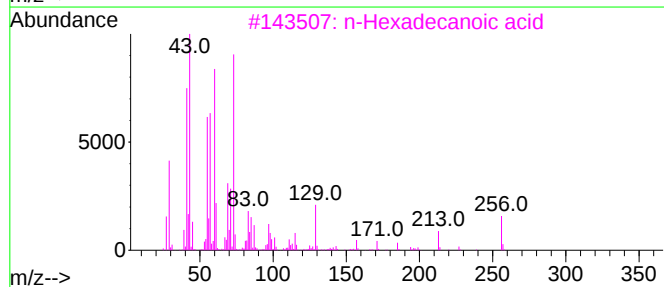
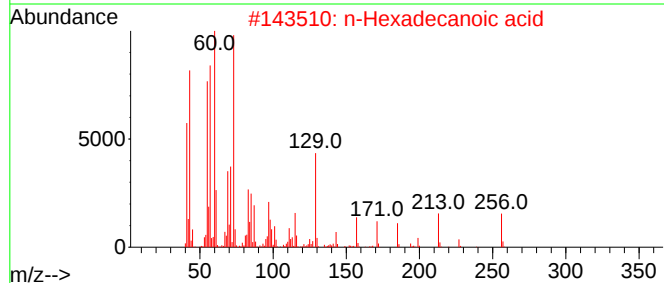
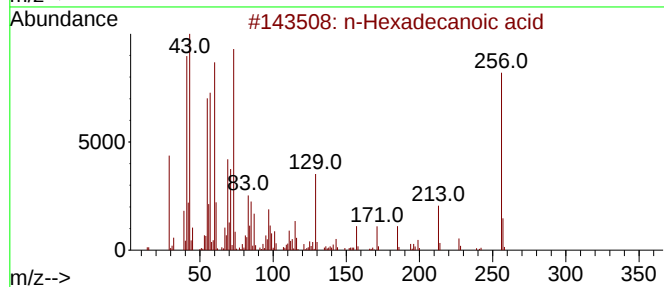
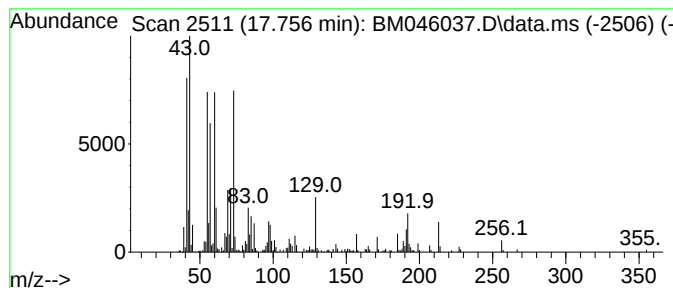
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.756	5.29 ng/ul	427610	Phenanthrene-d10	16.827

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4		Octadecanoic acid	284	C18H36O2	000057-11-4	87
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87



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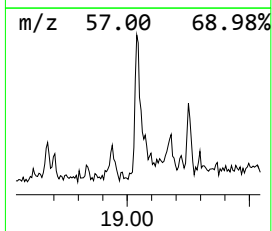
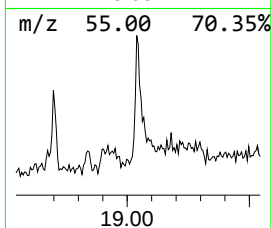
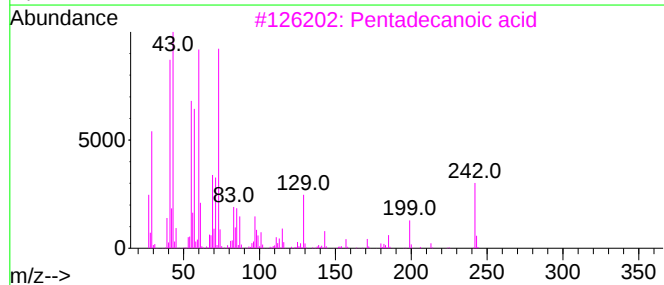
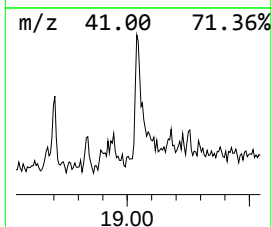
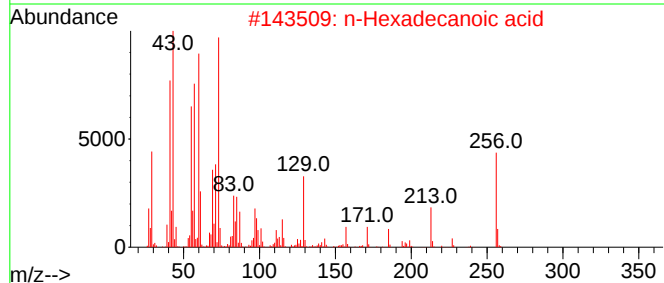
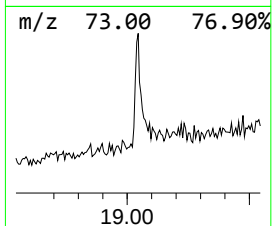
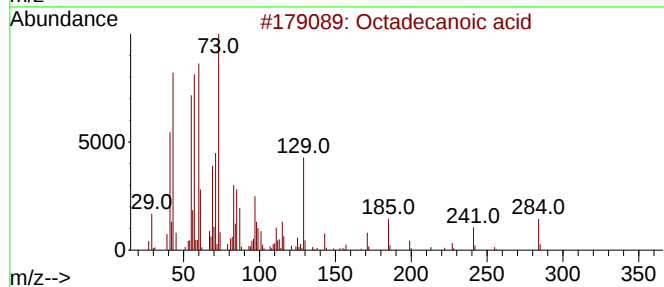
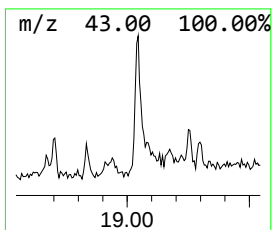
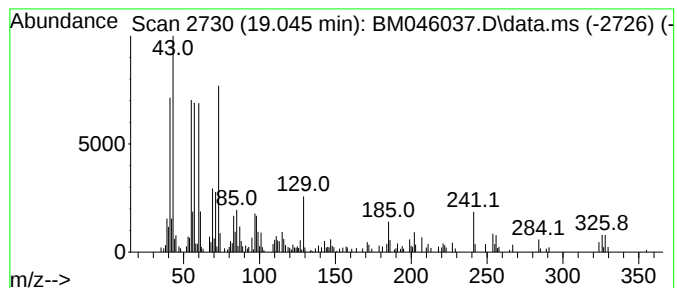
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.045	2.12 ng/ul	196488	Chrysene-d12	21.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061424\
Data File : BM046037.D
Acq On : 14 Jun 2024 13:43
Operator : MA/JU
Sample : P2695-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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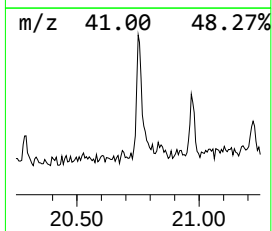
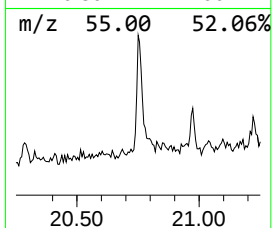
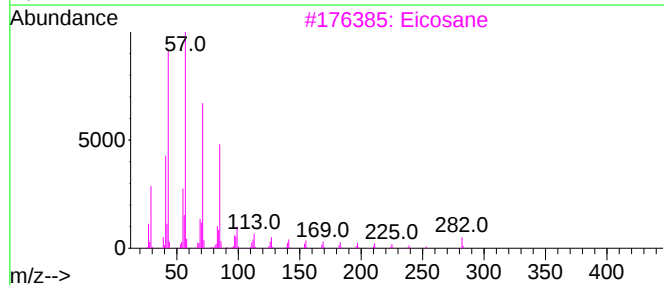
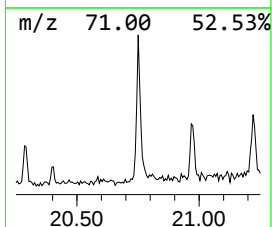
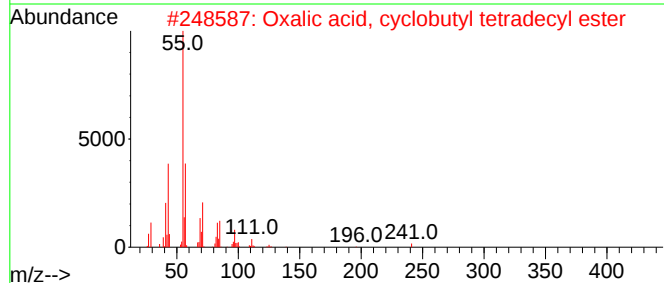
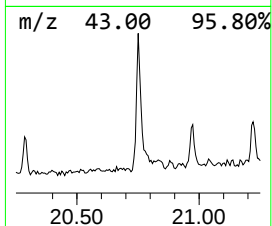
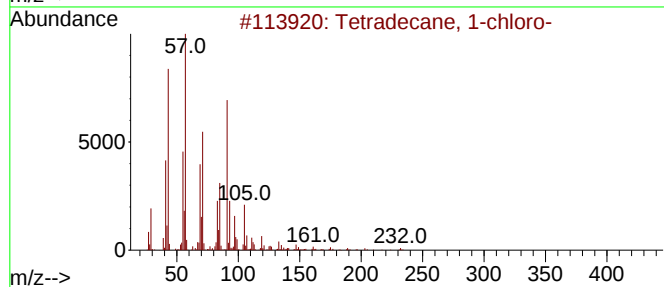
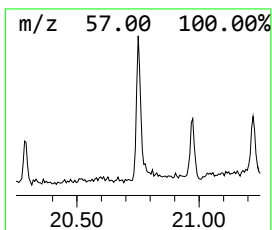
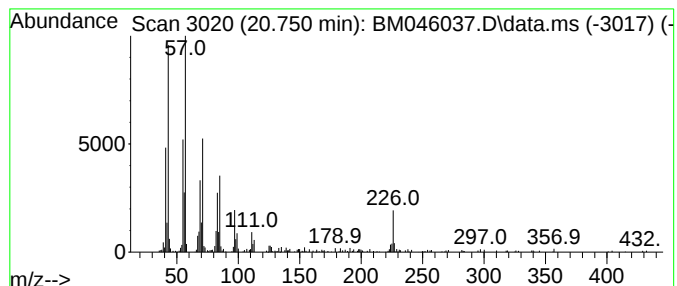
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Tetradecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.750	2.62 ng/ul	242164	Chrysene-d12	21.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	89
2			Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	80
3			Eicosane	282	C20H42	000112-95-8	78
4			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	74
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061424\
Data File : BM046037.D
Acq On : 14 Jun 2024 13:43
Operator : MA/JU
Sample : P2695-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4BJ9

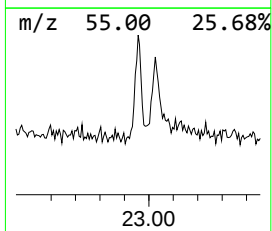
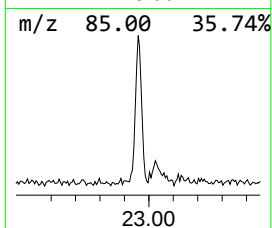
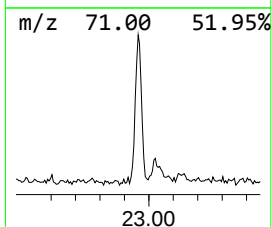
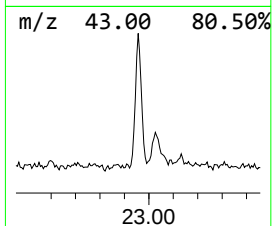
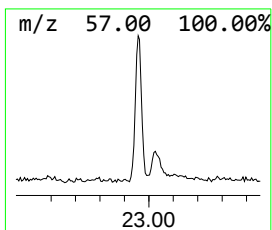
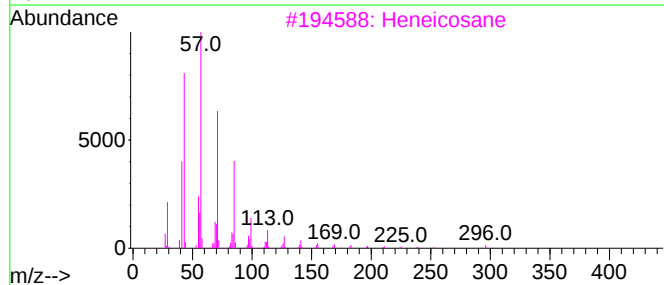
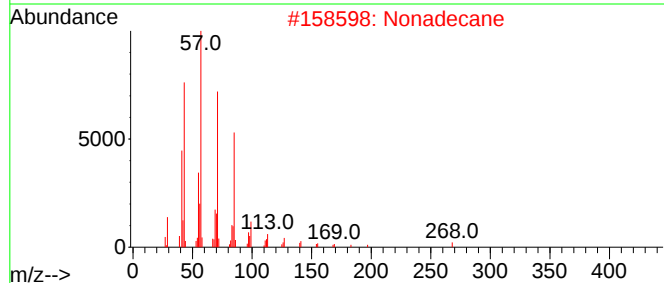
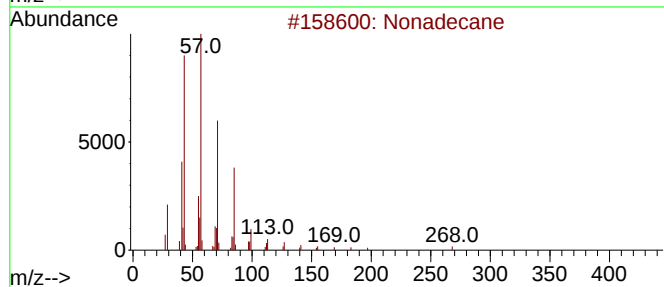
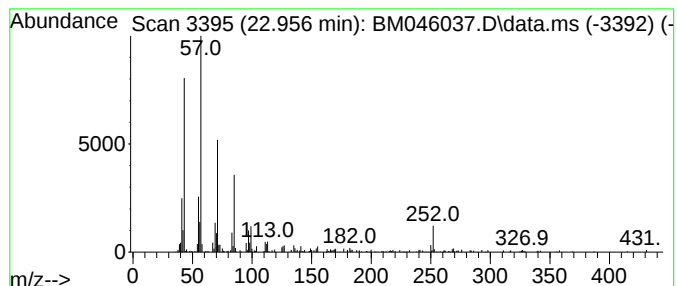
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.956	3.03 ng/ul	289124	Perylene-d12	23.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Nonadecane	268	C19H40	000629-92-5	92
3			Heneicosane	296	C21H44	000629-94-7	90
4			Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061424\
Data File : BM046037.D
Acq On : 14 Jun 2024 13:43
Operator : MA/JU
Sample : P2695-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A4BJ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM053124.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	4.622	3.2	ng/ul	136531	1	7.434	857717	20.0
n-Hexadecanoic ...	17.756	5.3	ng/ul	427610	4	16.827	1616220	20.0
Octadecanoic acid	19.045	2.1	ng/ul	196488	5	21.039	1851890	20.0
Tetradecane, 1-...	20.750	2.6	ng/ul	242164	5	21.039	1851890	20.0
(DEL) Alkane: S...	22.956	3.0	ng/ul	289124	6	23.744	1910130	20.0