

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
 Data File : BM036591.D
 Acq On : 19 Sep 2022 21:48
 Operator : CG/JU
 Sample : N4604-19
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A5779

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-BM091522.M
 Title : SVOA CALIBRATION

Signal : TIC: BM036591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.122	3	6	32	rVB	12311734	17713161	100.00%	15.165%
2	3.393	48	52	57	rBV	65741	86972	0.49%	0.074%
3	3.934	140	144	150	rBV	43595	54720	0.31%	0.047%
4	4.069	161	167	173	rVV	79071	129680	0.73%	0.111%
5	4.163	176	183	189	rBV2	35707	59212	0.33%	0.051%
6	5.104	337	343	347	rBV2	58901	98268	0.55%	0.084%
7	6.992	660	664	672	rBV5	14537	35011	0.20%	0.030%
8	7.175	687	695	704	rBV	1200000	1911956	10.79%	1.637%
9	7.351	717	725	734	rBV	1029875	1562879	8.82%	1.338%
10	7.551	751	759	767	rBV	1215232	1891521	10.68%	1.619%
11	7.645	773	775	783	rVB3	18155	41783	0.24%	0.036%
12	8.028	832	840	846	rVV	1490384	2365641	13.36%	2.025%
13	8.092	846	851	855	rVB2	16518	27318	0.15%	0.023%
14	8.728	950	959	969	rBV	1300862	2035045	11.49%	1.742%
15	8.857	975	981	988	rVB	24317	43957	0.25%	0.038%
16	9.192	1031	1038	1047	rBV	1131983	1847793	10.43%	1.582%
17	9.628	1105	1112	1119	rVB3	33543	64130	0.36%	0.055%
18	9.916	1154	1161	1173	rBV	857730	1416783	8.00%	1.213%
19	10.039	1178	1182	1189	rVV7	14631	34972	0.20%	0.030%
20	10.451	1245	1252	1261	rBV	1425659	2327267	13.14%	1.992%
21	10.610	1273	1279	1292	rBV	1091039	1683861	9.51%	1.442%
22	10.839	1308	1318	1325	rBV	2181106	3640309	20.55%	3.117%
23	10.892	1325	1327	1332	rVB	25631	30445	0.17%	0.026%
24	10.969	1332	1340	1353	rBV	755607	1344234	7.59%	1.151%
25	11.616	1444	1450	1458	rBV	12902	27787	0.16%	0.024%
26	11.863	1487	1492	1497	rBV3	20669	36881	0.21%	0.032%
27	12.257	1555	1559	1564	rBV2	25872	38932	0.22%	0.033%
28	12.416	1579	1586	1591	rVV	29923	55754	0.31%	0.048%
29	12.492	1594	1599	1604	rVB	35891	55979	0.32%	0.048%
30	12.704	1629	1635	1641	rVB	30504	51403	0.29%	0.044%
31	13.268	1725	1731	1737	rVB4	20331	31629	0.18%	0.027%
32	13.486	1764	1768	1774	rBV	59426	81113	0.46%	0.069%
33	13.557	1774	1780	1787	rBV2	48812	88165	0.50%	0.075%
34	13.816	1817	1824	1831	rBV4	14302	39529	0.22%	0.034%
35	13.974	1846	1851	1855	rBV3	33057	48856	0.28%	0.042%
36	14.063	1855	1866	1876	rVV	2581973	3555931	20.08%	3.044%

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37	14.139	1876	1879	1883	rVB4	23016	27273	0.15%	0.023%
38	14.345	1908	1914	1925	rVB	2999292	4336678	24.48%	3.713%
39	14.551	1945	1949	1955	rVB2	29106	39354	0.22%	0.034%
40	14.651	1957	1966	1973	rBV	3489468	4961853	28.01%	4.248%
41	14.827	1989	1996	2012	rBV	1068626	1603453	9.05%	1.373%
42	14.986	2019	2023	2029	rBV6	22685	39548	0.22%	0.034%
43	15.057	2029	2035	2041	rVV4	67227	119958	0.68%	0.103%
44	15.268	2062	2071	2076	rBV6	17210	38929	0.22%	0.033%
45	15.439	2092	2100	2107	rBV7	29426	75002	0.42%	0.064%
46	15.498	2107	2110	2115	rVB2	31019	42871	0.24%	0.037%
47	15.639	2126	2134	2140	rBV	3791936	5478612	30.93%	4.690%
48	15.745	2146	2152	2161	rBV	889354	1201548	6.78%	1.029%
49	15.874	2170	2174	2177	rBV	29750	42516	0.24%	0.036%
50	15.986	2189	2193	2198	rVB3	22703	35561	0.20%	0.030%
51	16.080	2205	2209	2214	rVV5	19933	28988	0.16%	0.025%
52	16.133	2214	2218	2224	rVB3	18949	35059	0.20%	0.030%
53	16.204	2229	2230	2239	rVB6	17245	29933	0.17%	0.026%
54	16.362	2253	2257	2258	rVV2	41548	56518	0.32%	0.048%
55	16.380	2258	2260	2264	rVV	48640	61563	0.35%	0.053%
56	16.521	2281	2284	2291	rVB8	14575	27532	0.16%	0.024%
57	16.927	2349	2353	2357	rVV3	52423	69812	0.39%	0.060%
58	17.151	2388	2391	2397	rVV2	37757	60992	0.34%	0.052%
59	17.204	2397	2400	2404	rVB5	26321	31757	0.18%	0.027%
60	17.386	2424	2431	2436	rBV	4156767	5800509	32.75%	4.966%
61	17.427	2436	2438	2442	rVV	176783	203046	1.15%	0.174%
62	17.486	2442	2448	2458	rVV	3856825	5589407	31.56%	4.785%
63	17.568	2459	2462	2468	rVB6	29769	50105	0.28%	0.043%
64	17.768	2492	2496	2501	rBV5	13530	28221	0.16%	0.024%
65	17.892	2513	2517	2520	rBV2	23699	31544	0.18%	0.027%
66	17.962	2525	2529	2533	rBV2	27881	35513	0.20%	0.030%
67	18.062	2541	2546	2550	rBV	250094	304603	1.72%	0.261%
68	18.280	2576	2583	2592	rBV3	398404	802976	4.53%	0.687%
69	18.445	2607	2611	2616	rVV2	62326	116511	0.66%	0.100%
70	18.492	2616	2619	2622	rVB	48705	56960	0.32%	0.049%
71	18.580	2630	2634	2636	rBV	41907	55668	0.31%	0.048%
72	18.756	2660	2664	2667	rBV	53872	68156	0.38%	0.058%
73	18.898	2685	2688	2692	rVB	26625	34443	0.19%	0.029%
74	19.162	2729	2733	2738	rBV2	137568	213080	1.20%	0.182%
75	19.227	2738	2744	2748	rVB3	131047	213431	1.20%	0.183%
76	19.309	2754	2758	2759	rBV2	41809	53639	0.30%	0.046%

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77	19.327	2759	2761	2764	rVB	42973	55941	0.32%	0.048%
78	19.398	2770	2773	2775	rBV	56987	78070	0.44%	0.067%
79	19.433	2775	2779	2786	rVB	407765	537683	3.04%	0.460%
80	19.550	2795	2799	2807	rBV2	177776	267026	1.51%	0.229%
81	19.762	2829	2835	2849	rBV	5510020	7753032	43.77%	6.638%
82	20.280	2919	2923	2926	rBV3	100603	131046	0.74%	0.112%
83	20.315	2926	2929	2933	rVB	133753	140602	0.79%	0.120%
84	20.386	2938	2941	2945	rBV3	54350	72204	0.41%	0.062%
85	20.762	3001	3005	3010	rBV	275695	339560	1.92%	0.291%
86	20.803	3010	3012	3016	rVB	84015	88591	0.50%	0.076%
87	21.262	3086	3090	3097	rBV	1638627	2050355	11.58%	1.755%
88	21.544	3132	3138	3143	rBV	5287192	7097631	40.07%	6.077%
89	21.715	3164	3167	3171	rBV	237221	283136	1.60%	0.242%
90	22.197	3243	3249	3260	rBV	1600511	2440380	13.78%	2.089%
91	22.462	3291	3294	3303	rVB2	233481	316329	1.79%	0.271%
92	22.697	3331	3334	3336	rBV	130000	157406	0.89%	0.135%
93	22.950	3373	3377	3387	rVB	421347	665739	3.76%	0.570%
94	23.262	3427	3430	3434	rBV	358698	572594	3.23%	0.490%
95	23.309	3434	3438	3452	rVB2	1058634	1830568	10.33%	1.567%
96	23.833	3520	3527	3534	rBV2	3336077	6486405	36.62%	5.553%
97	23.991	3547	3554	3567	rVB2	3145865	6309273	35.62%	5.402%
98	24.268	3598	3601	3609	rVB3	210619	382890	2.16%	0.328%
99	24.662	3662	3668	3675	rVB2	525945	1080292	6.10%	0.925%
100	24.744	3677	3682	3694	rVB2	468272	1004828	5.67%	0.860%

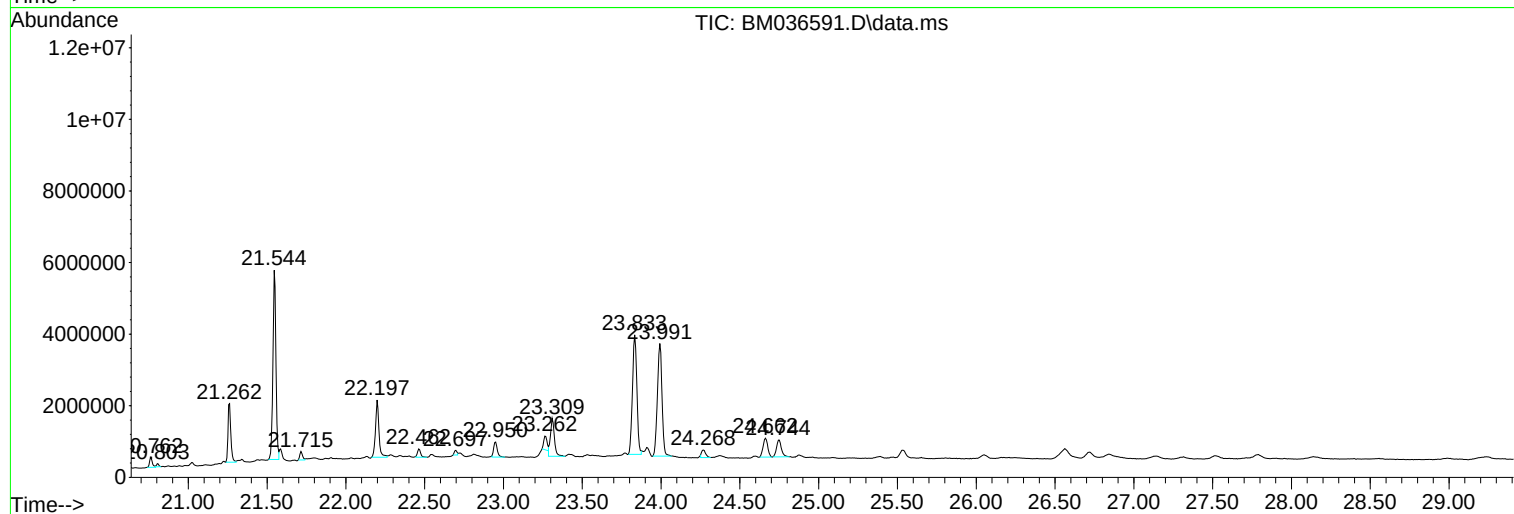
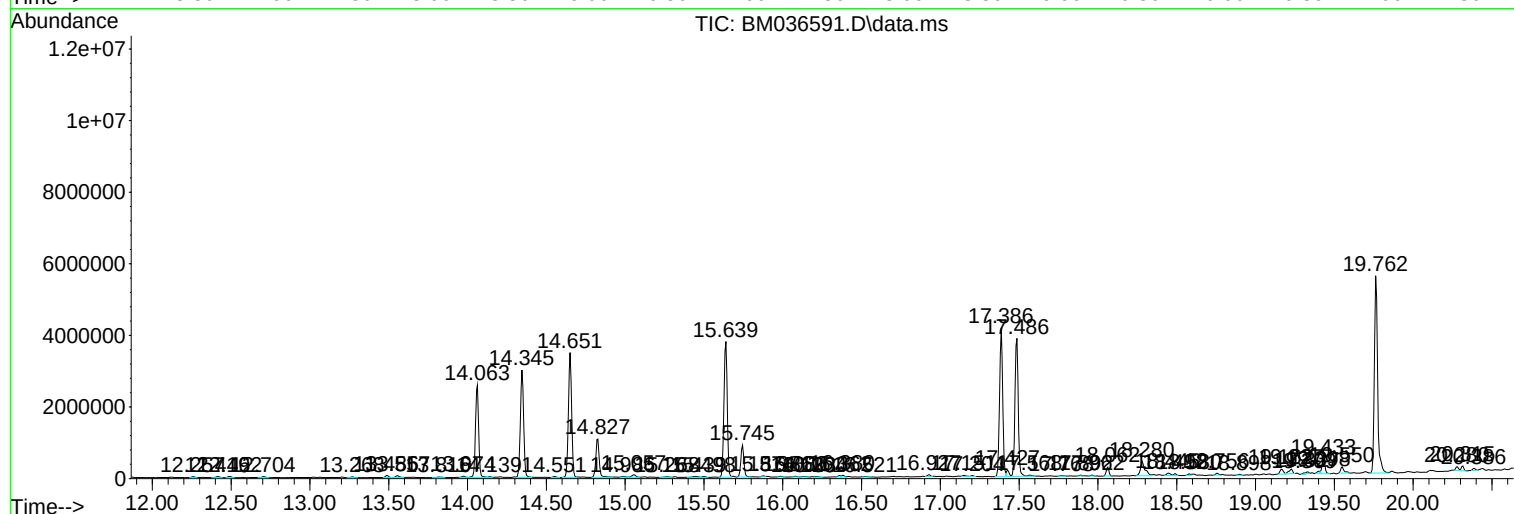
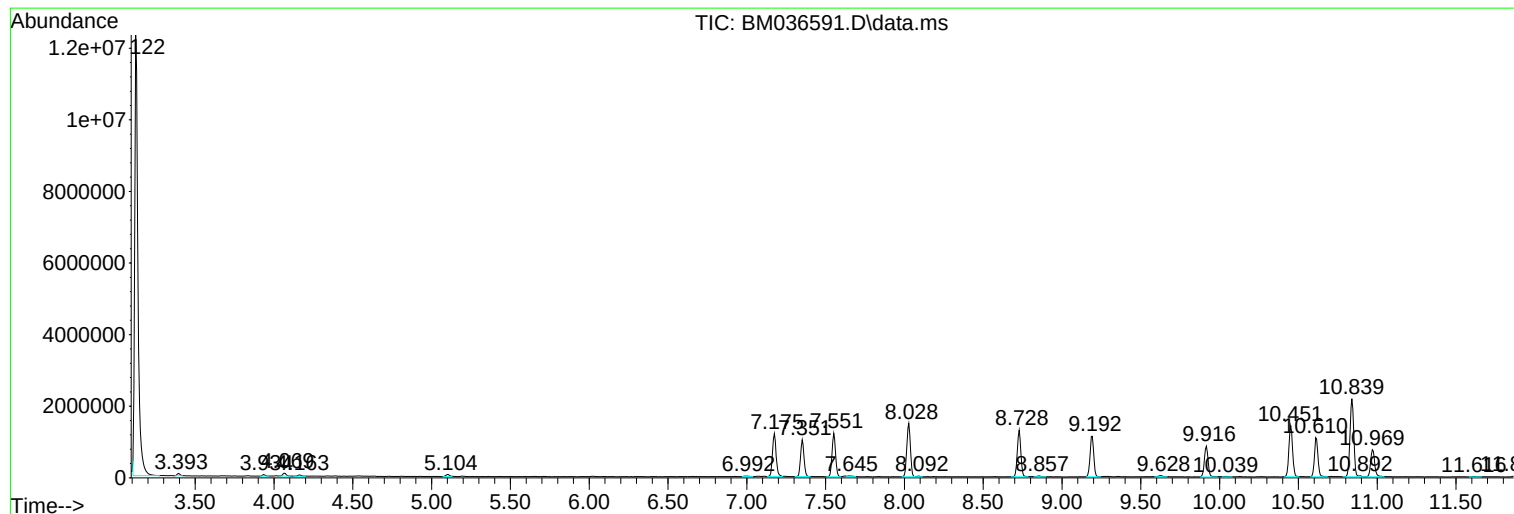
Sum of corrected areas: 116803580

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

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



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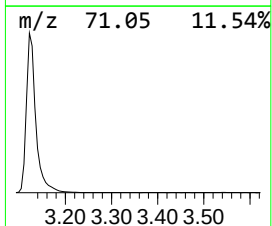
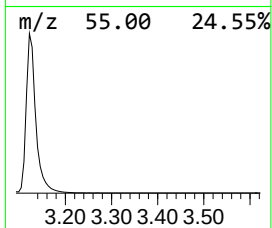
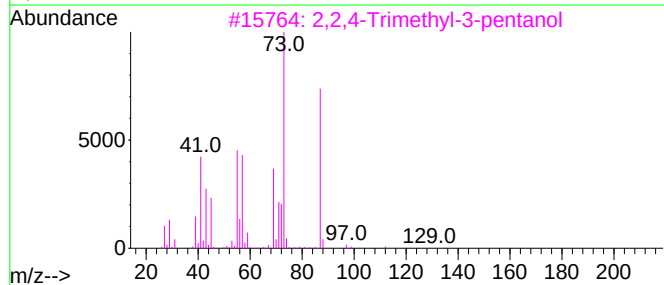
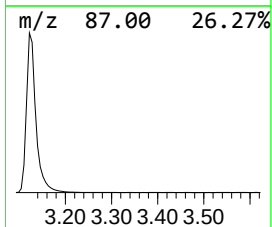
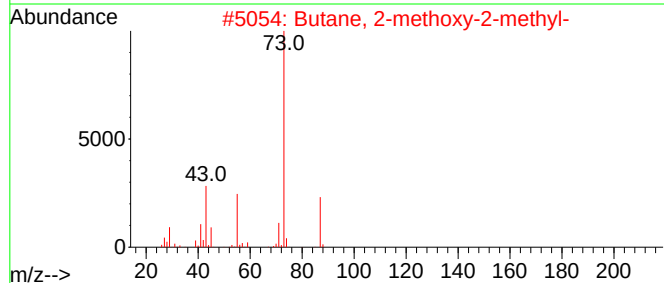
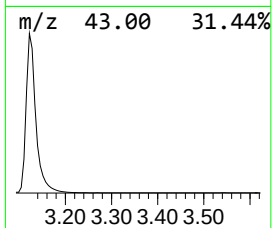
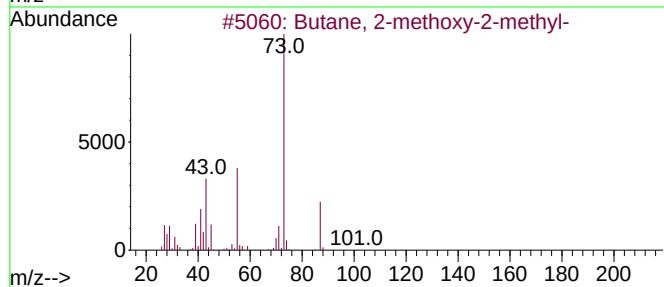
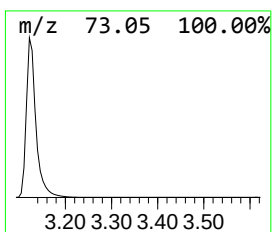
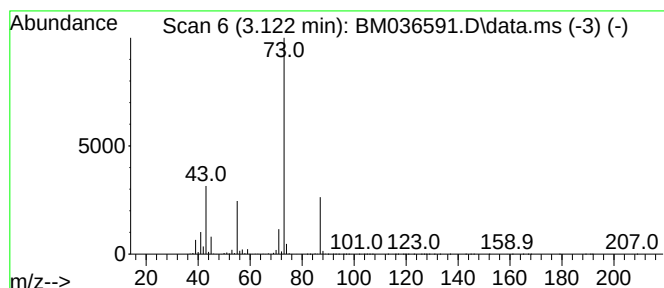
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	149.75 ng/ul	17713200	1,4-Dichlorobenzene-d4	8.028

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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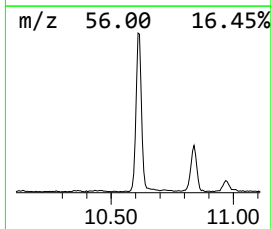
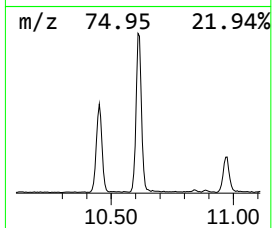
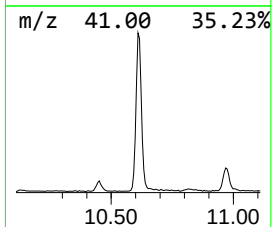
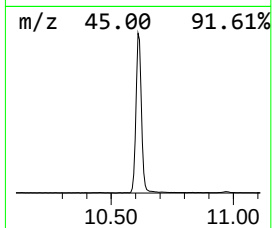
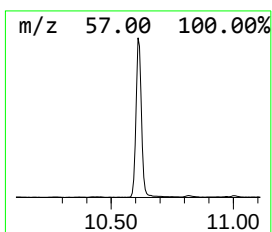
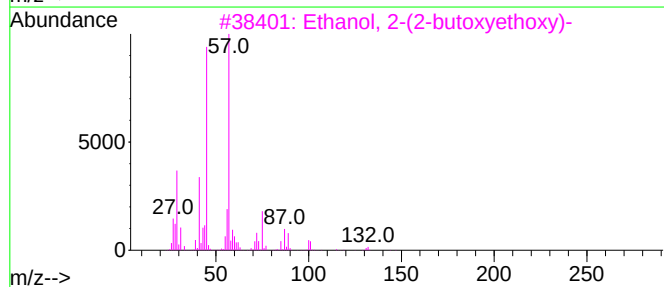
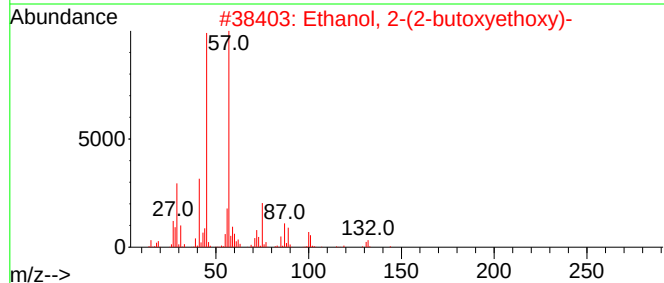
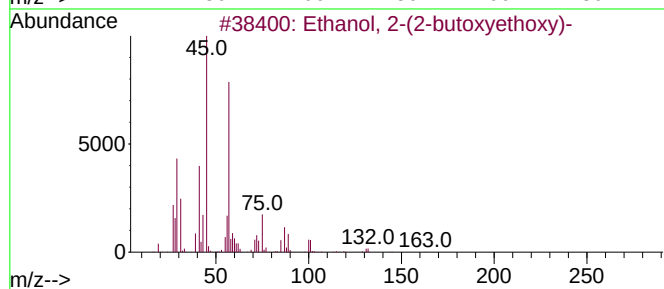
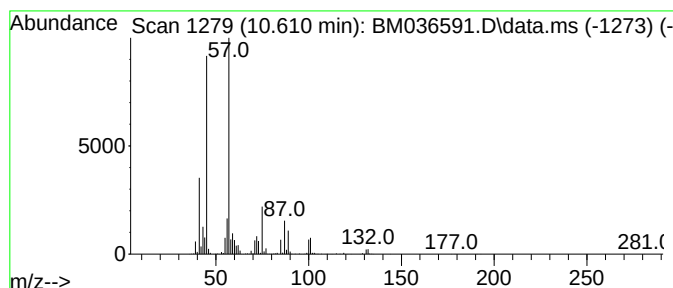
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	9.25 ng/ul	1683860	Naphthalene-d8	10.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83



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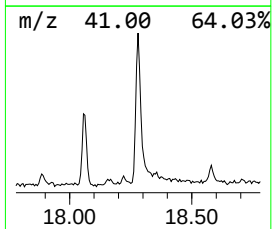
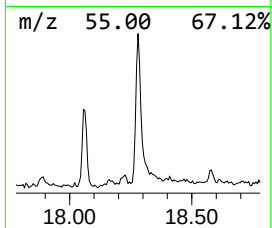
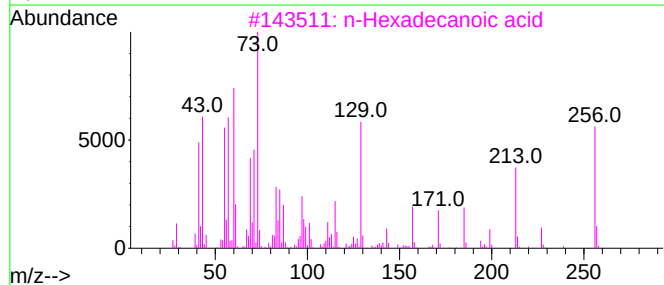
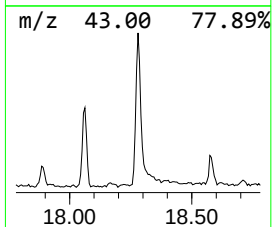
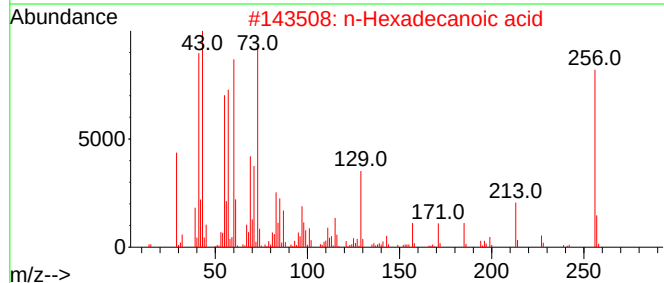
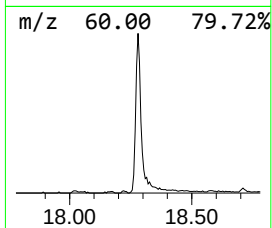
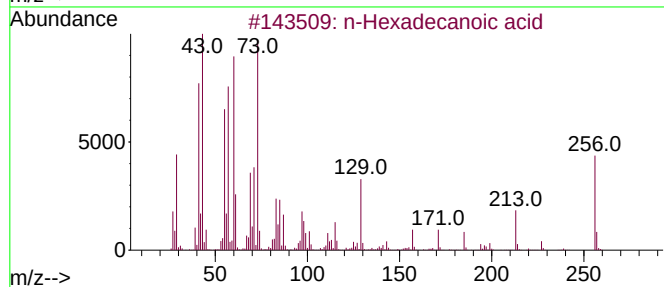
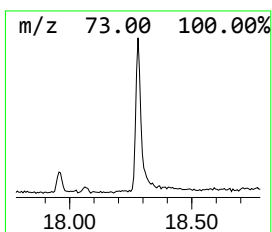
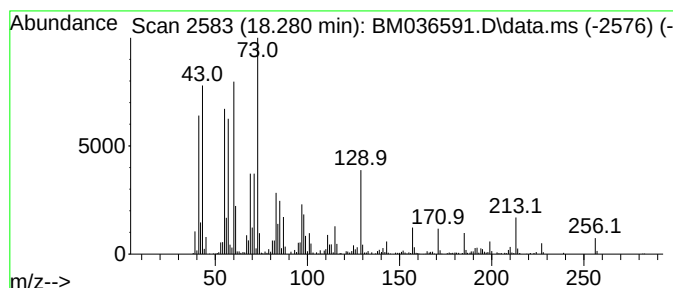
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.280	2.77 ng/ul	802976	Phenanthrene-d10	17.386

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	99
5			Tridecanoic acid	214	C13H26O2	000638-53-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
Data File : BM036591.D
Acq On : 19 Sep 2022 21:48
Operator : CG/JU
Sample : N4604-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

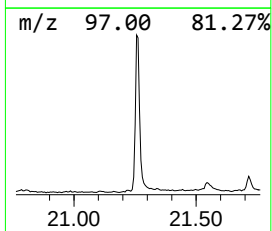
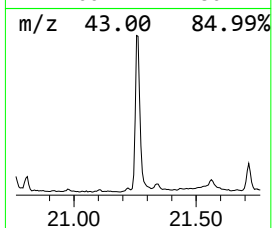
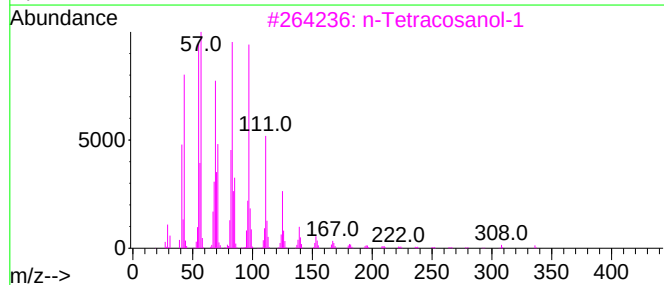
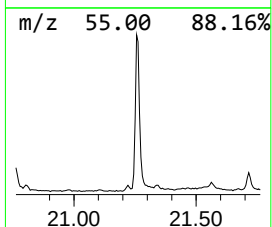
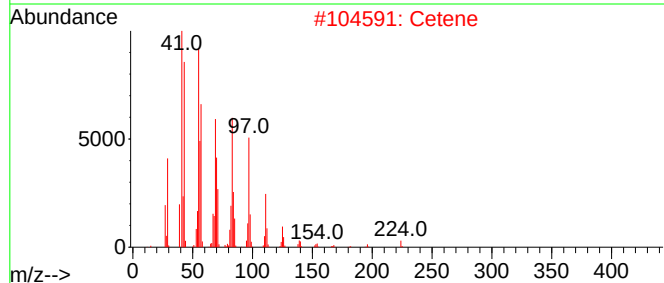
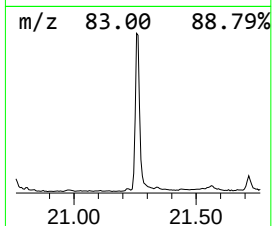
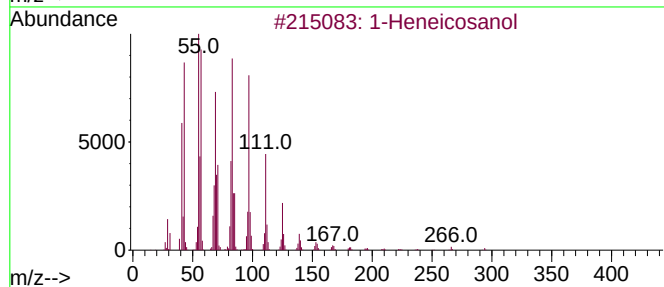
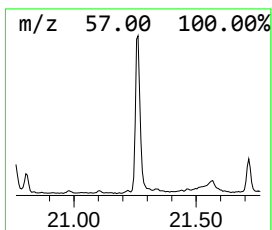
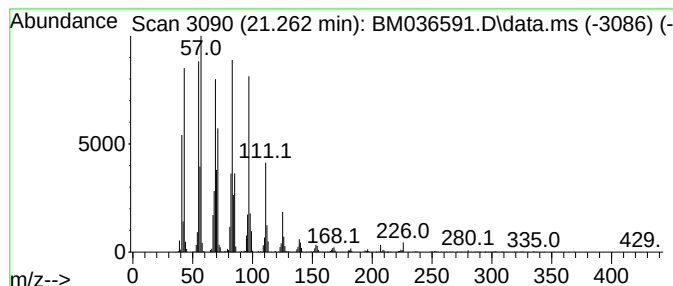
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.262	5.78 ng/ul	2050360	Chrysene-d12		21.544	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	Cetene		224	C16H32	000629-73-2	95
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
4	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94
5	Behenic alcohol		326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
Data File : BM036591.D
Acq On : 19 Sep 2022 21:48
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Sample : N4604-19
Misc :
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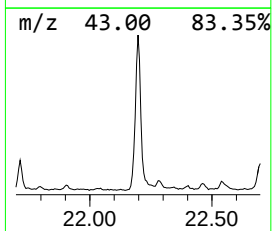
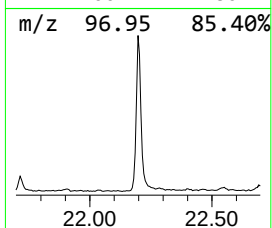
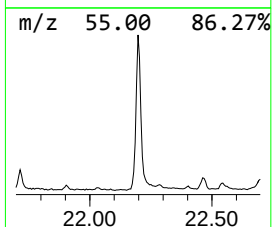
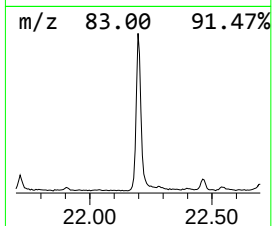
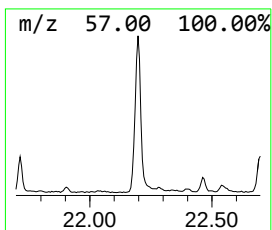
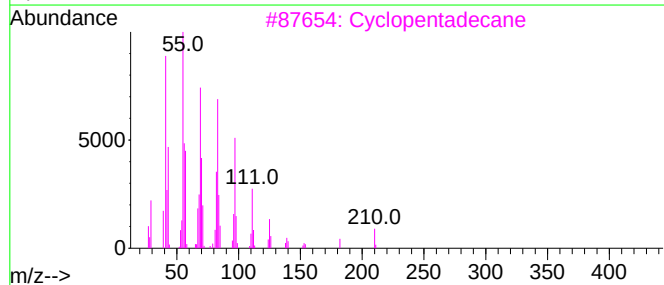
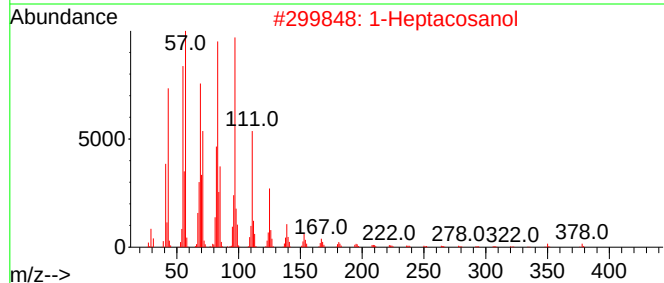
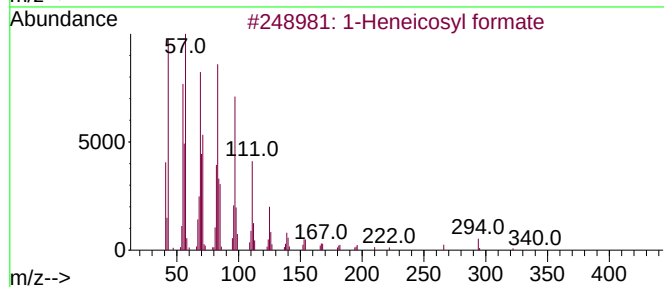
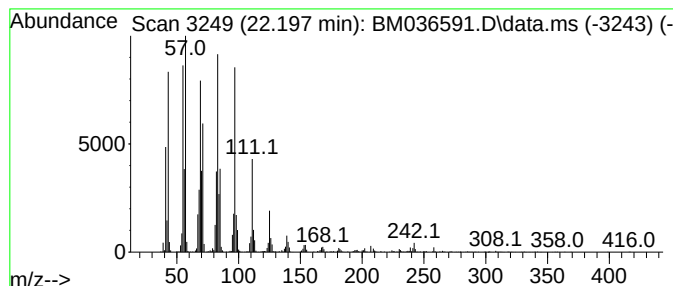
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.197	6.88 ng/ul	2440380	Chrysene-d12	21.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2			1-Heptacosanol	396	C27H56O	002004-39-9	93
3			Cyclopentadecane	210	C15H30	000295-48-7	93
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
Data File : BM036591.D
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Operator : CG/JU
Sample : N4604-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

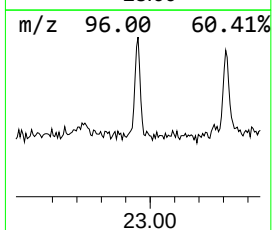
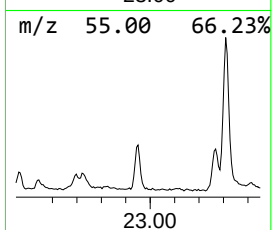
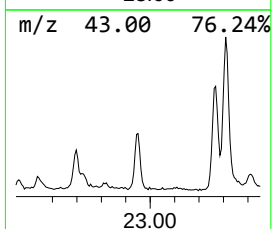
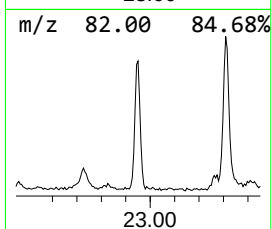
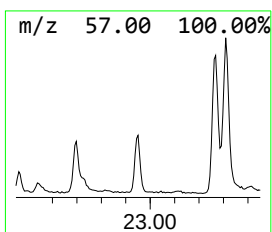
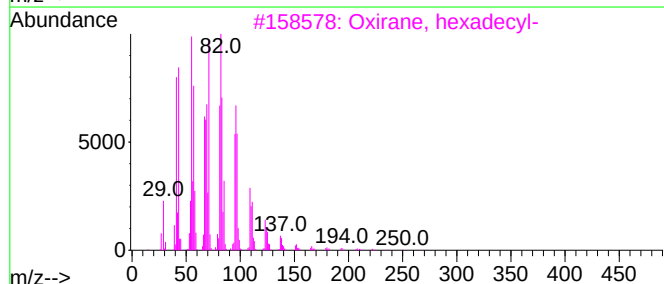
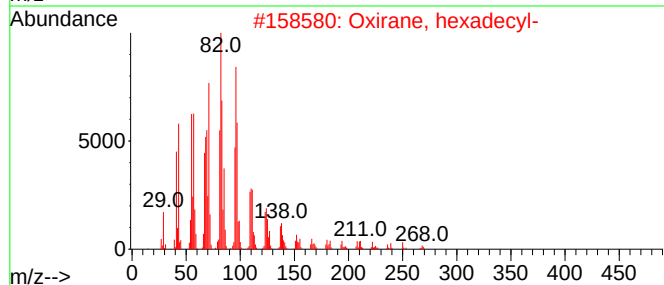
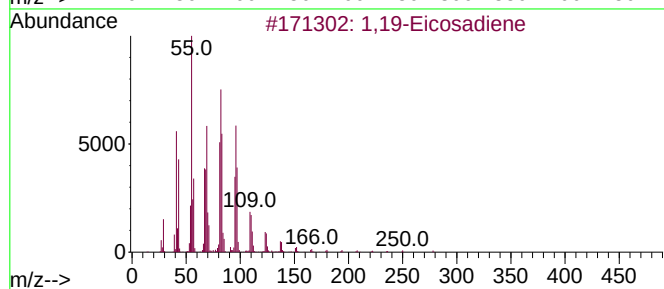
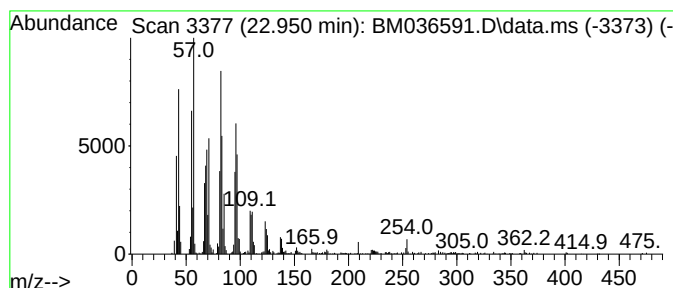
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 1,19-Eicosadiene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.950	2.11 ng/ul	665739	Perylene-d12	23.991	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5	Tetracosanal	352	C24H48O	057866-08-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
Data File : BM036591.D
Acq On : 19 Sep 2022 21:48
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Sample : N4604-19
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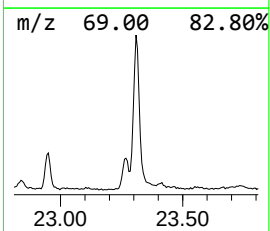
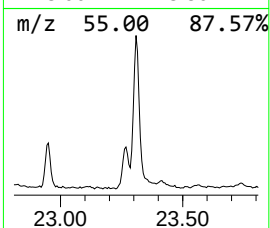
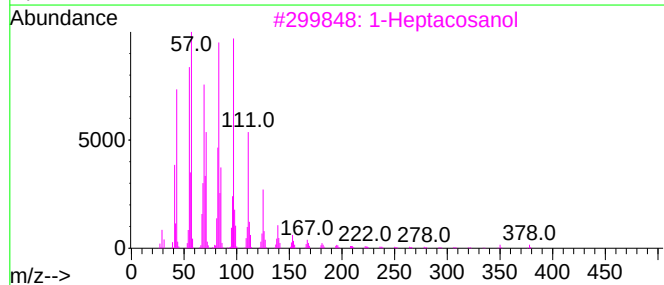
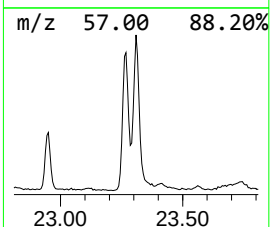
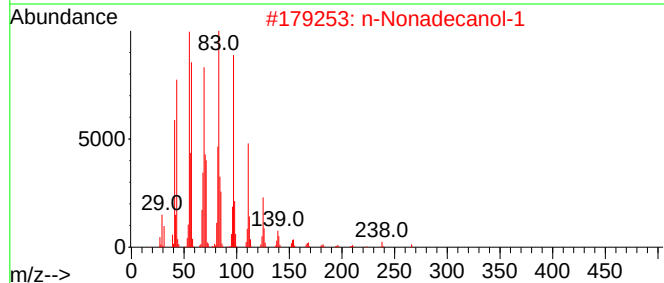
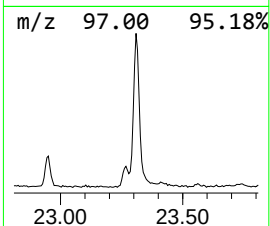
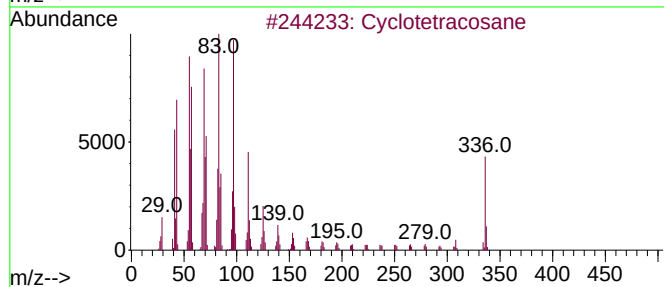
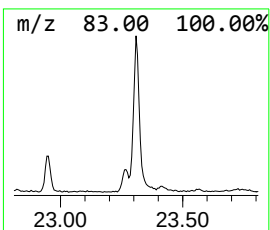
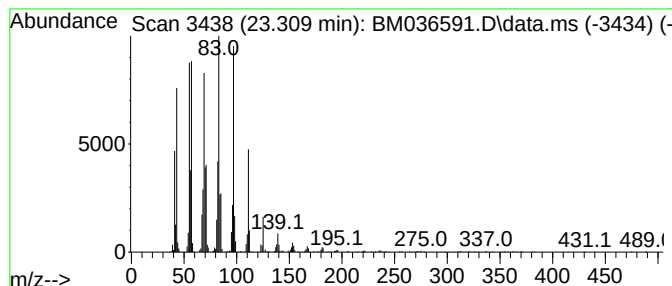
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Cyclic23.309 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.309	5.80 ng/ul	1830570	Perylene-d12	23.991

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	98
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	90
4			Fumaric acid, 2-chloroethyl hept...	416	C23H41ClO4	1000330-62-3	87
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
Data File : BM036591.D
Acq On : 19 Sep 2022 21:48
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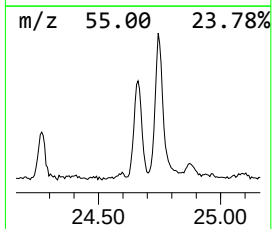
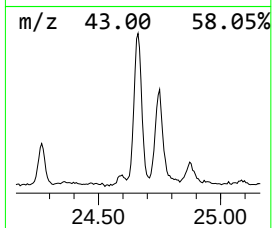
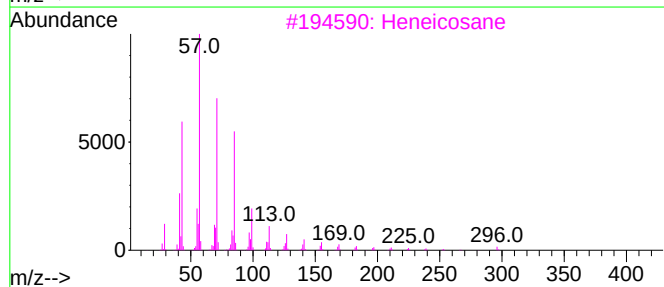
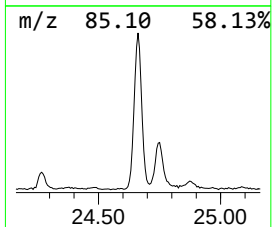
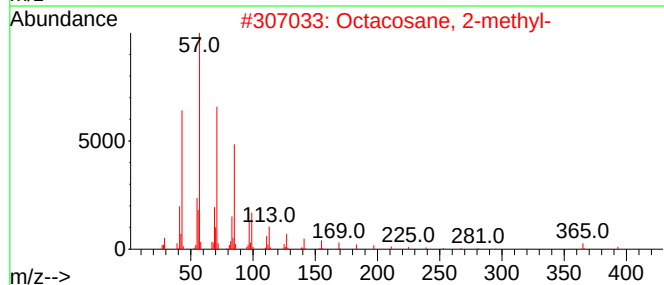
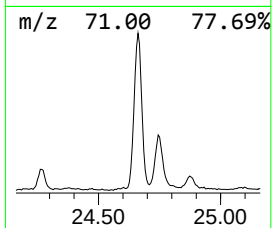
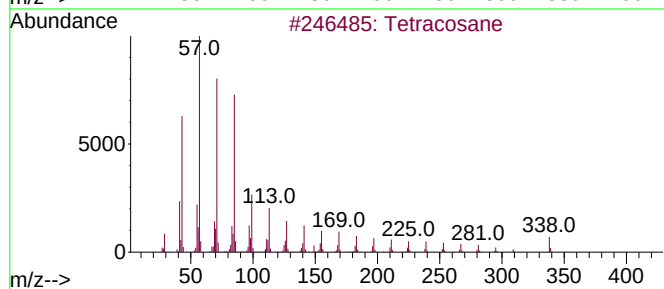
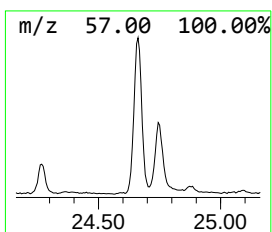
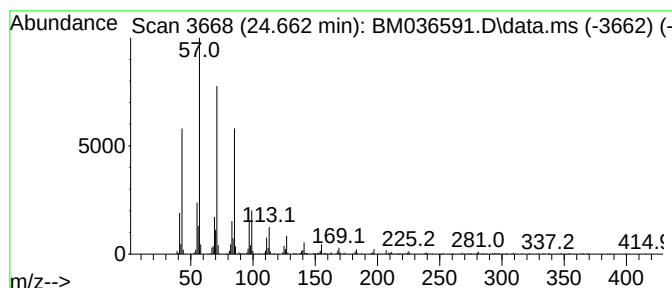
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.662	3.42 ng/ul	1080290	Perylene-d12	23.991

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	94
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
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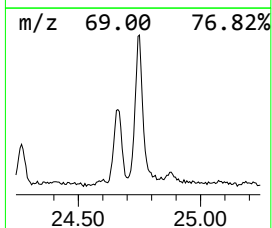
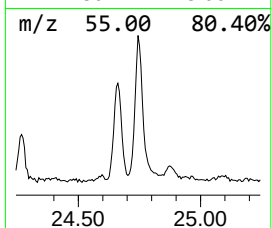
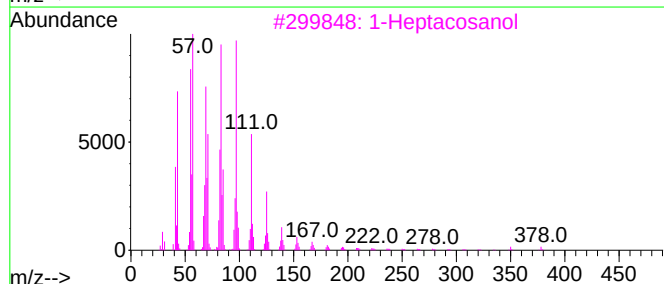
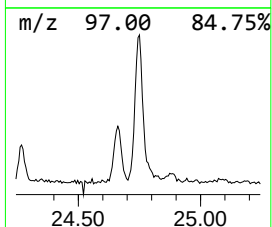
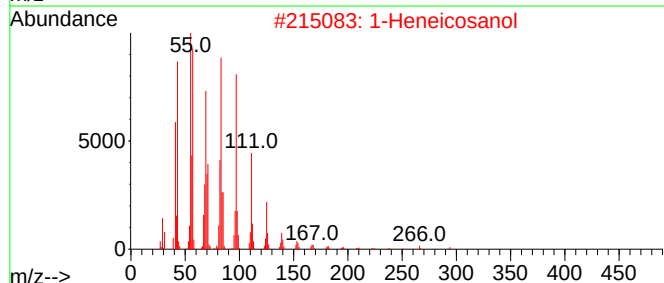
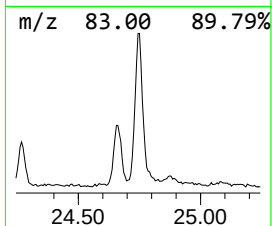
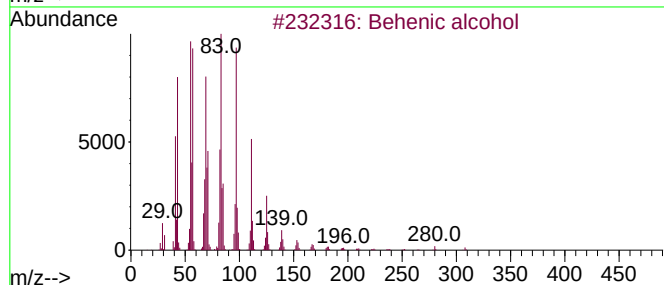
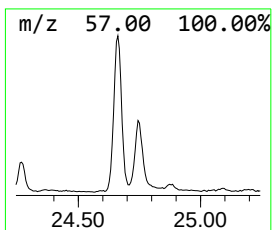
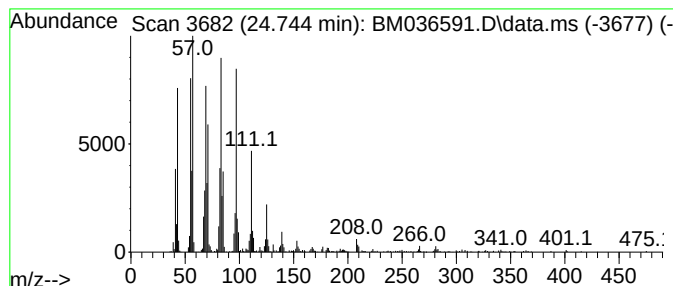
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.744	3.19 ng/ul	1004830	Perylene-d12	23.991

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			1-Heptacosanol	396	C27H56O	002004-39-9	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091922\
Data File : BM036591.D
Acq On : 19 Sep 2022 21:48
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Sample : N4604-19
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM091522.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
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Ethanol, 2-(2-b...	10.610	9.3	ng/ul	1683860	2	10.839	3640310	20.0
n-Hexadecanoic ...	18.280	2.8	ng/ul	802976	4	17.386	5800510	20.0
1-Heneicosanol	21.262	5.8	ng/ul	2050360	5	21.544	7097630	20.0
1-Heneicosyl fo...	22.197	6.9	ng/ul	2440380	5	21.544	7097630	20.0
1,19-Eicosadiene	22.950	2.1	ng/ul	665739	6	23.991	6309270	20.0
(DEL) Alkane: C...	23.309	5.8	ng/ul	1830570	6	23.991	6309270	20.0
(DEL) Alkane: S...	24.662	3.4	ng/ul	1080290	6	23.991	6309270	20.0
Behenic alcohol	24.744	3.2	ng/ul	1004830	6	23.991	6309270	20.0