

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043405.D
 Acq On : 18 Dec 2023 22:22
 Operator : MA/JU
 Sample : 05807-05
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AX7

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-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043405.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	47	rVB	177387	244562	1.13%	0.148%
2	3.669	79	82	85	rBV	264830	381632	1.76%	0.232%
3	3.710	86	89	102	rVB	300275	583441	2.69%	0.354%
4	3.810	102	106	133	rVB	2142811	3340226	15.40%	2.027%
5	4.298	137	189	192	rBV	2547741	21688768	100.00%	13.162%
6	4.863	278	285	297	rVB	168391	273614	1.26%	0.166%
7	4.993	301	307	313	rVV	102830	157131	0.72%	0.095%
8	5.075	317	321	330	rVB	20844	38241	0.18%	0.023%
9	5.287	350	357	364	rVB	456158	702709	3.24%	0.426%
10	5.428	376	381	385	rBV	42926	64296	0.30%	0.039%
11	6.063	484	489	496	rVB2	34921	55711	0.26%	0.034%
12	6.981	640	645	650	rBV	53322	87589	0.40%	0.053%
13	7.157	668	675	688	rVB	2830466	4605780	21.24%	2.795%
14	7.334	698	705	717	rVB	2182887	3486516	16.08%	2.116%
15	7.522	729	737	747	rBV	2682379	4323613	19.93%	2.624%
16	7.616	747	753	758	rVV2	22496	41751	0.19%	0.025%
17	7.992	810	817	827	rBV	2040333	3284767	15.15%	1.993%
18	8.075	827	831	838	rVB2	35902	66624	0.31%	0.040%
19	8.704	929	938	945	rBV	3408456	5556115	25.62%	3.372%
20	8.763	945	948	954	rVB2	29859	46088	0.21%	0.028%
21	9.163	1008	1016	1028	rBV	2530478	4347590	20.05%	2.638%
22	9.545	1074	1081	1089	rBV2	23031	46603	0.21%	0.028%
23	9.733	1106	1113	1123	rBV	154282	243309	1.12%	0.148%
24	9.886	1130	1139	1152	rBV	2245079	3692213	17.02%	2.241%
25	10.022	1157	1162	1167	rBV5	14251	29111	0.13%	0.018%
26	10.422	1221	1230	1242	rBV	3183264	5342033	24.63%	3.242%
27	10.804	1284	1295	1304	rBV	2743906	4727188	21.80%	2.869%
28	10.945	1311	1319	1336	rBV	3188861	5459153	25.17%	3.313%
29	11.351	1380	1388	1395	rBV4	50399	127447	0.59%	0.077%
30	11.551	1414	1422	1433	rBV	203577	380499	1.75%	0.231%
31	11.710	1446	1449	1459	rVB	10796	23572	0.11%	0.014%
32	12.216	1528	1535	1542	rBV2	40076	66105	0.30%	0.040%
33	12.380	1559	1563	1570	rVB2	52217	87117	0.40%	0.053%
34	12.598	1592	1600	1604	rBV2	26448	50810	0.23%	0.031%
35	13.021	1667	1672	1680	rVB8	13298	26606	0.12%	0.016%
36	13.451	1735	1745	1748	rBV	52877	91920	0.42%	0.056%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.1 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	13.521	1754	1757	1763	rVB	24043	35985	0.17%	0.022%
38	13.604	1765	1771	1778	rVV7	13227	29370	0.14%	0.018%
39	14.045	1838	1846	1855	rVV	4818133	6710978	30.94%	4.073%
40	14.321	1886	1893	1904	rVB	5725659	8661516	39.94%	5.256%
41	14.621	1936	1944	1952	rBV	3588536	5391299	24.86%	3.272%
42	14.821	1970	1978	1995	rBV	2325576	3675094	16.94%	2.230%
43	15.039	2009	2015	2024	rVB7	32489	69386	0.32%	0.042%
44	15.615	2106	2113	2127	rVB	6743290	9618747	44.35%	5.837%
45	15.733	2127	2133	2145	rBV	1889302	2607445	12.02%	1.582%
46	15.851	2147	2153	2162	rVB2	34804	71653	0.33%	0.043%
47	16.327	2228	2234	2241	rVB8	16073	33286	0.15%	0.020%
48	16.392	2241	2245	2251	rVB5	27090	43877	0.20%	0.027%
49	16.556	2269	2273	2276	rBV4	15758	26810	0.12%	0.016%
50	16.821	2314	2318	2324	rVB2	19444	35067	0.16%	0.021%
51	17.127	2366	2370	2373	rBV5	17872	26788	0.12%	0.016%
52	17.368	2404	2411	2417	rBV	3640405	5142590	23.71%	3.121%
53	17.468	2420	2428	2437	rVV	6485155	8989764	41.45%	5.456%
54	17.562	2441	2444	2449	rVV5	35800	46913	0.22%	0.028%
55	17.751	2471	2476	2484	rVB4	45477	77062	0.36%	0.047%
56	18.039	2522	2525	2530	rVB7	17082	25510	0.12%	0.015%
57	18.268	2558	2564	2579	rBV	890624	1469678	6.78%	0.892%
58	18.598	2616	2620	2625	rVB6	27197	42569	0.20%	0.026%
59	18.698	2633	2637	2641	rVB	78441	94767	0.44%	0.058%
60	19.315	2738	2742	2748	rBV3	71311	100116	0.46%	0.061%
61	19.392	2750	2755	2758	rBV2	96500	149241	0.69%	0.091%
62	19.539	2775	2780	2791	rBV	209523	376722	1.74%	0.229%
63	19.750	2810	2816	2823	rBV	6623145	8731934	40.26%	5.299%
64	19.803	2823	2825	2830	rVB2	39515	44365	0.20%	0.027%
65	20.268	2901	2904	2908	rBV2	106417	146246	0.67%	0.089%
66	20.303	2908	2910	2915	rVB2	71984	77564	0.36%	0.047%
67	20.756	2984	2987	2990	rBV	105915	109269	0.50%	0.066%
68	20.797	2992	2994	2998	rVB	92805	103851	0.48%	0.063%
69	21.256	3068	3072	3082	rBV	1399659	1993643	9.19%	1.210%
70	21.439	3091	3103	3116	rBV	2208563	8064005	37.18%	4.894%
71	21.539	3116	3120	3133	rVB2	3308032	4618200	21.29%	2.803%
72	21.715	3147	3150	3155	rVB	127000	146745	0.68%	0.089%
73	22.197	3227	3232	3244	rVB4	249713	552222	2.55%	0.335%
74	23.809	3499	3506	3517	rVB2	4401854	8332449	38.42%	5.057%
75	23.968	3526	3533	3542	rVB	2192957	4540022	20.93%	2.755%

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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-BM121523.MA.M
Title : SVOA CALIBRATION

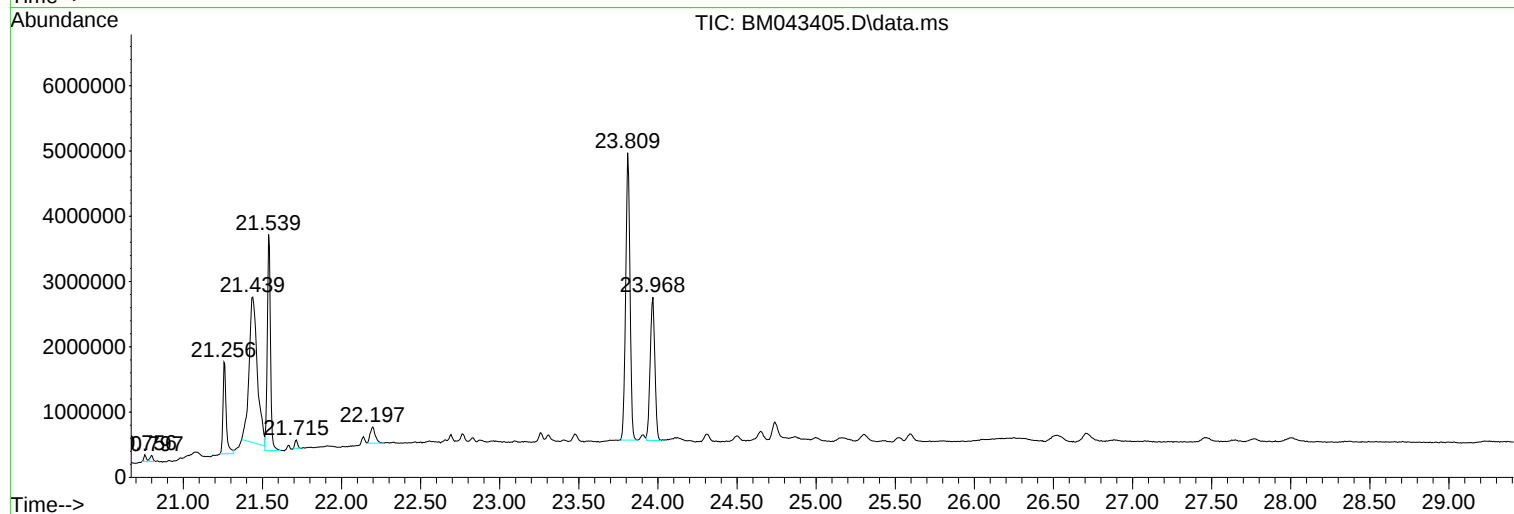
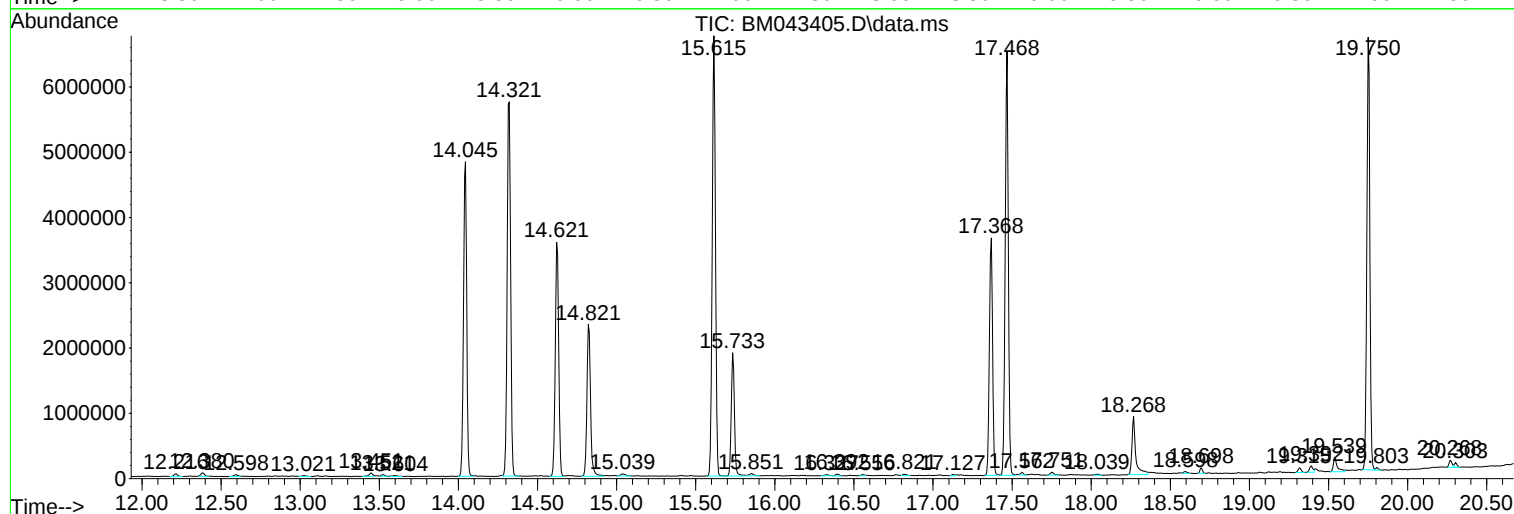
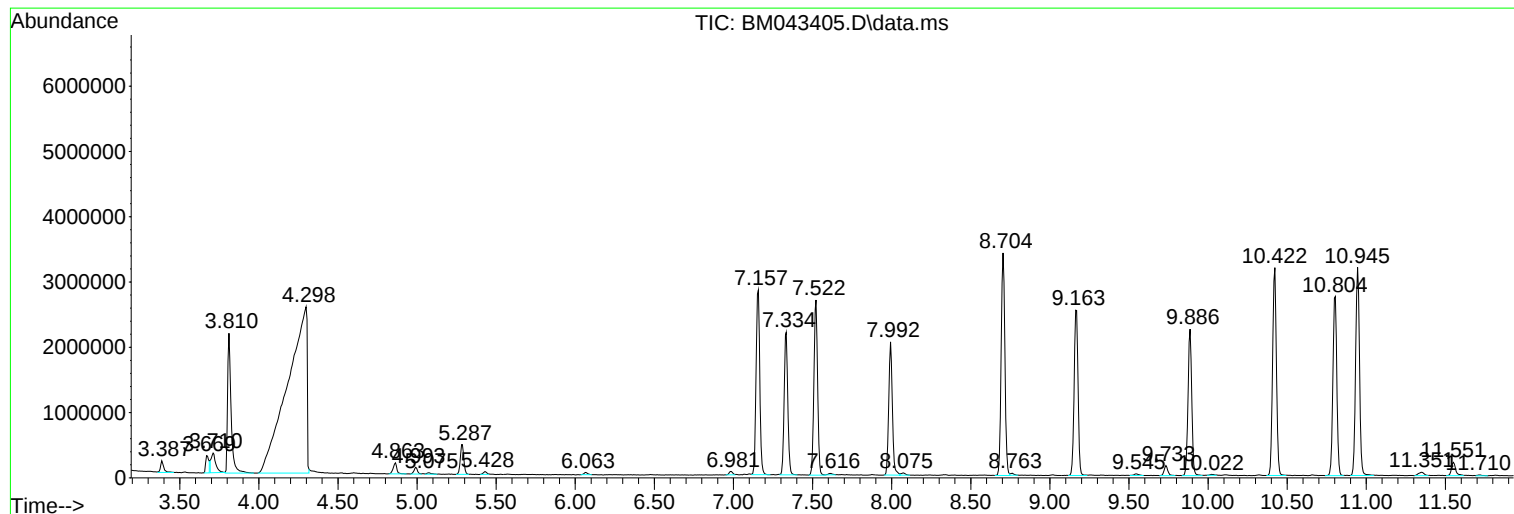
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
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Instrument :
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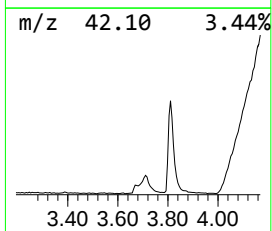
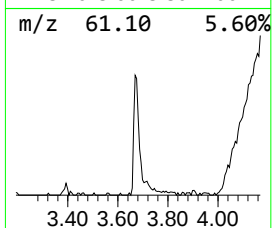
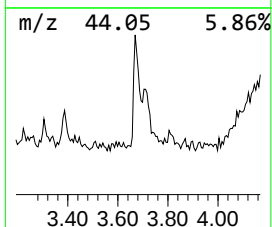
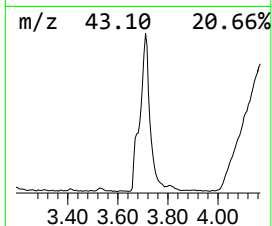
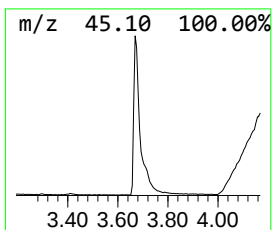
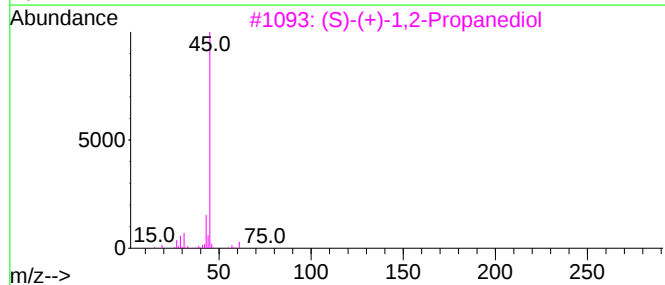
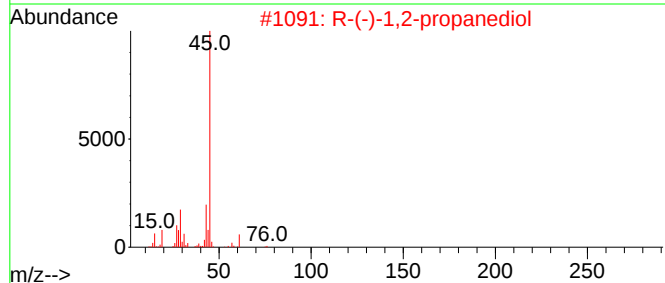
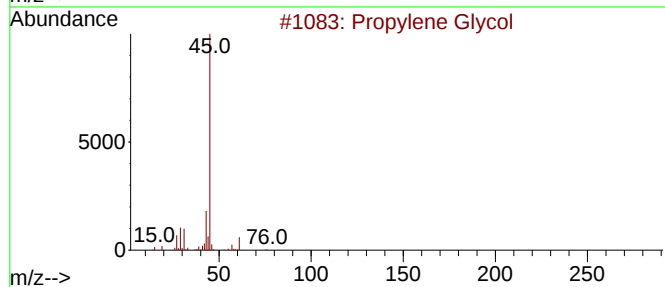
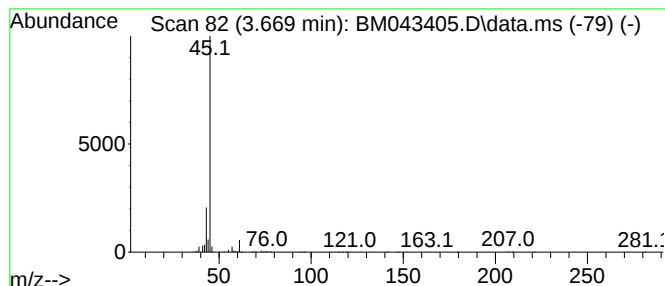
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	2.32 ng/ul	381632	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4			2-Propanol, 1-hydrazino-	90	C3H10N2O	018501-20-7	9
5			2-Pentanol	88	C5H12O	006032-29-7	9



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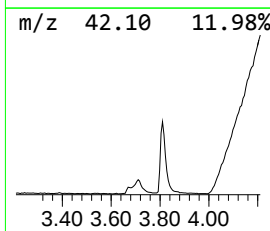
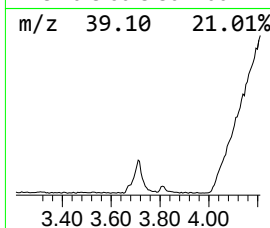
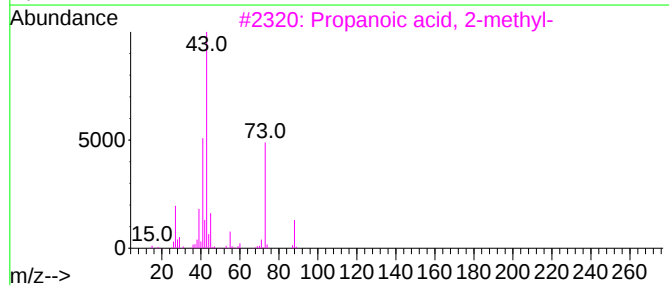
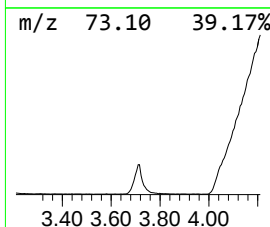
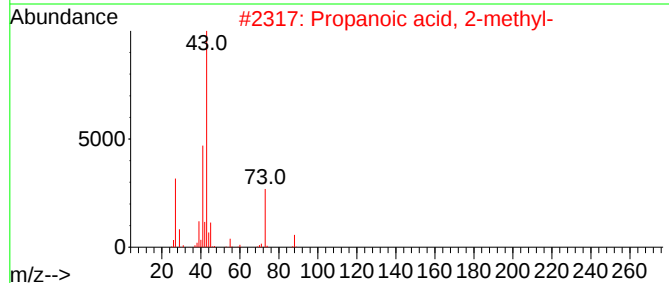
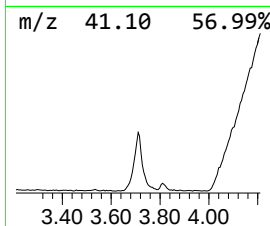
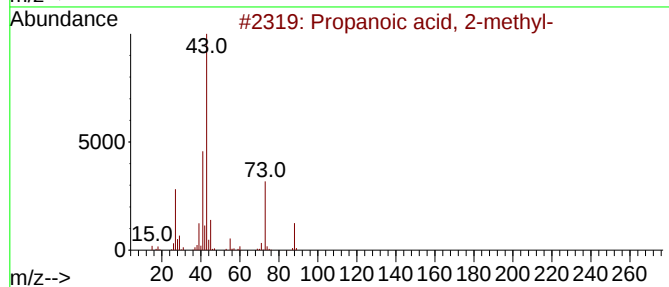
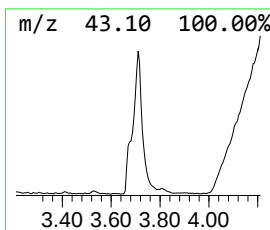
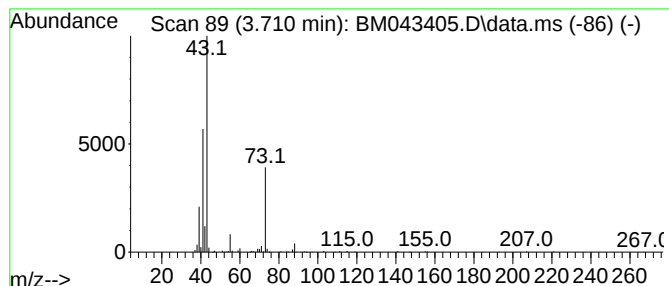
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Propanoic acid, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.710	3.55 ng/ul	583441	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	83
2			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	72
3			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	64
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	38
5			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	37



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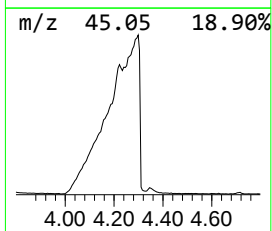
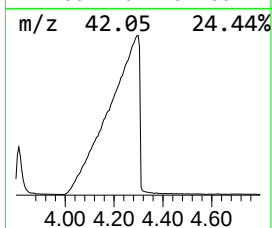
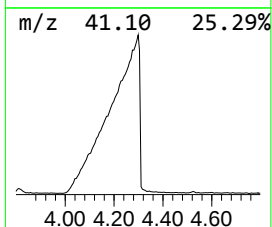
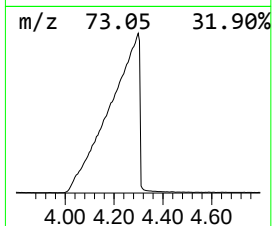
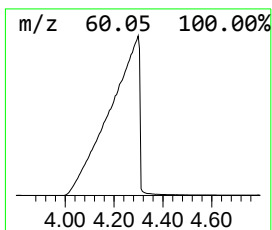
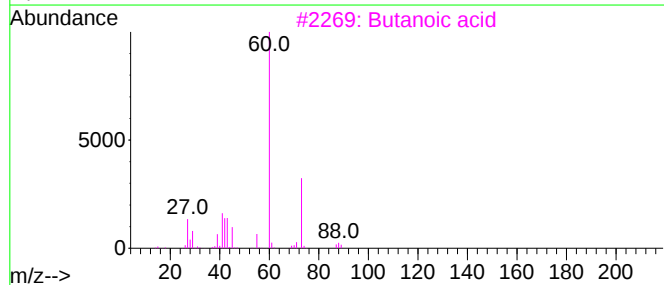
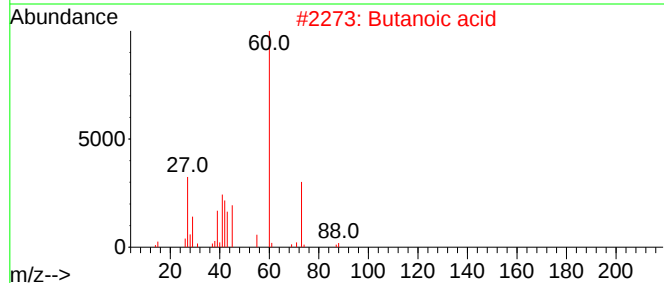
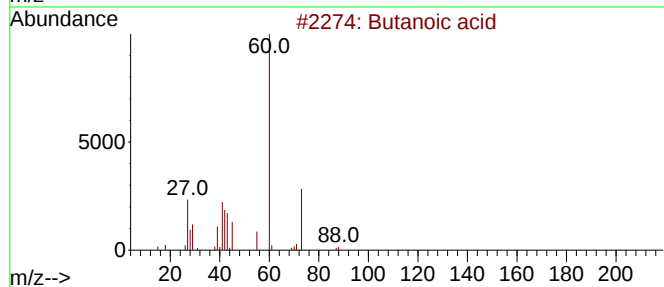
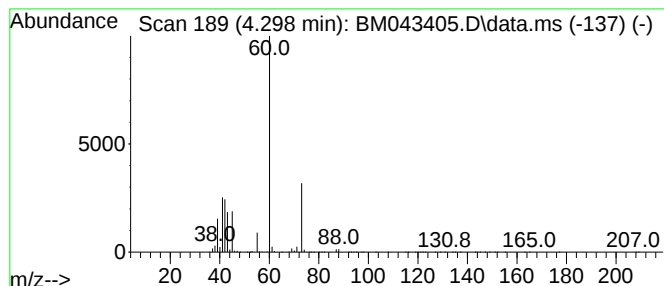
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.298	132.06 ng/ul	21688800	1,4-Dichlorobenzene-d4	7.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Butanoic acid	88	C4H8O2	000107-92-6	90
3			Butanoic acid	88	C4H8O2	000107-92-6	86
4			Butanoic acid	88	C4H8O2	000107-92-6	80
5			Pentanoic acid	102	C5H10O2	000109-52-4	45



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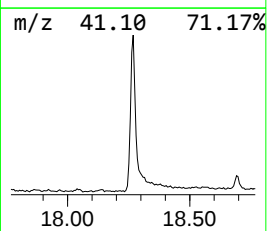
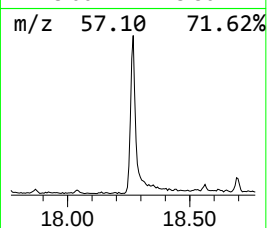
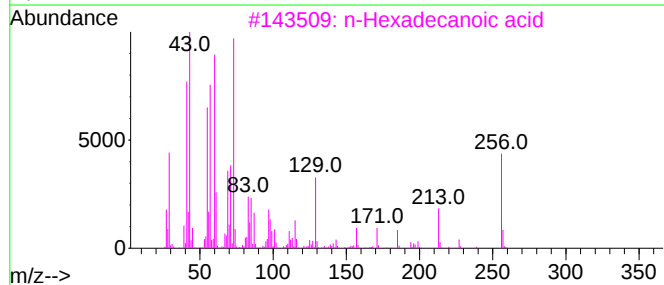
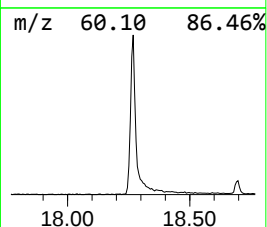
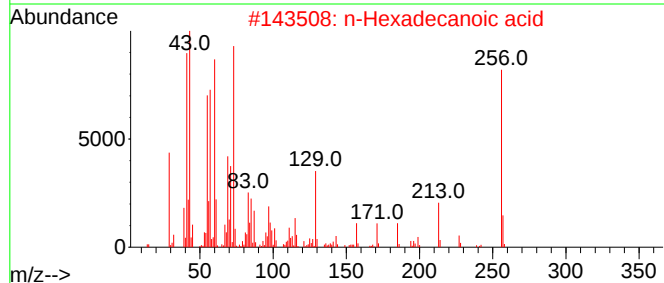
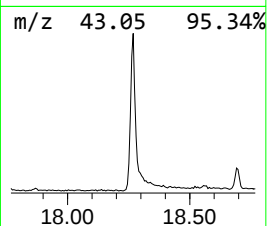
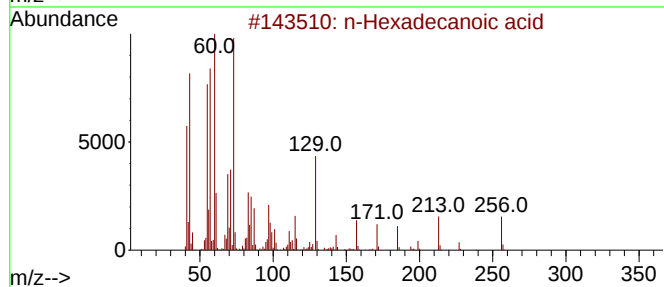
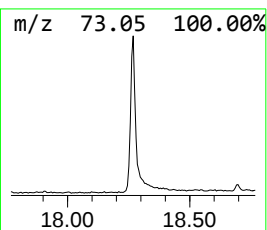
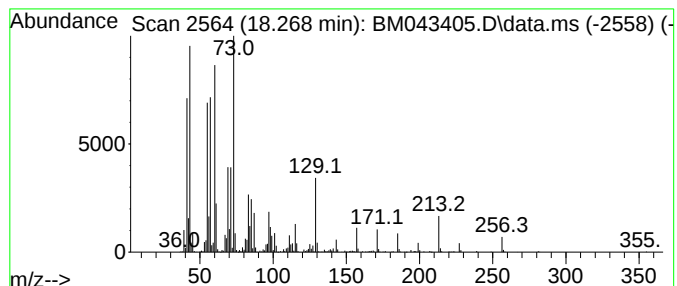
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	5.72 ng/ul	1469680	Phenanthrene-d10	17.368

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	98
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043405.D
Acq On : 18 Dec 2023 22:22
Operator : MA/JU
Sample : 05807-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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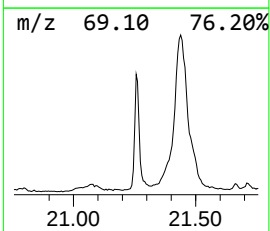
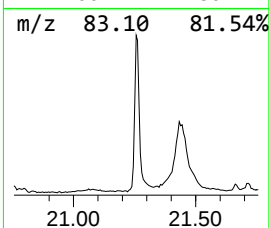
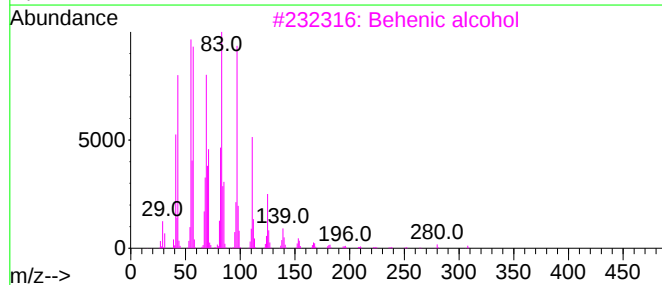
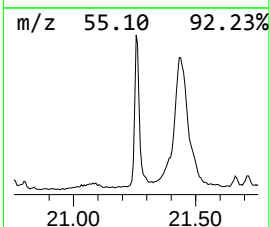
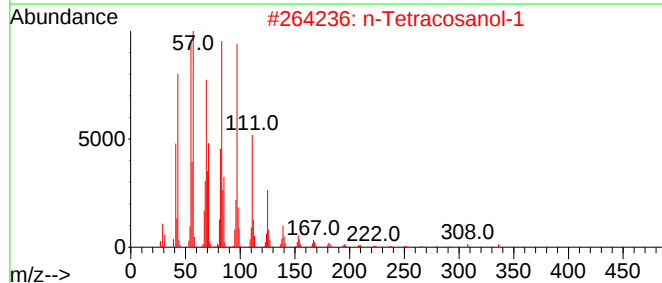
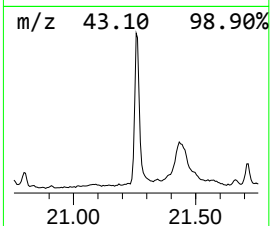
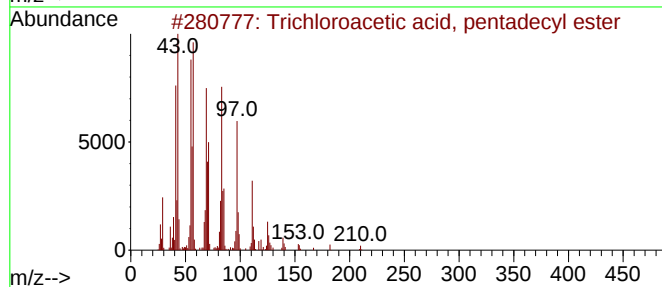
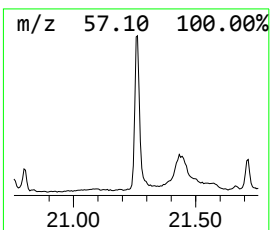
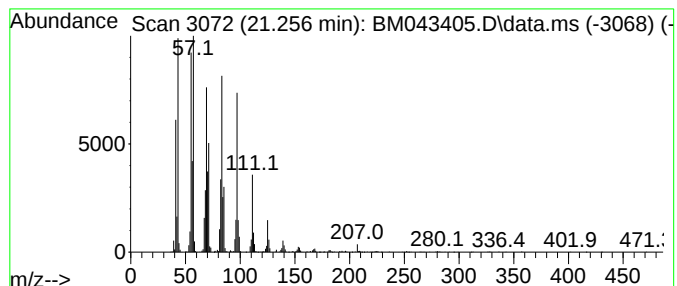
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.256	8.63 ng/ul	1993640	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043405.D
Acq On : 18 Dec 2023 22:22
Operator : MA/JU
Sample : 05807-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX7

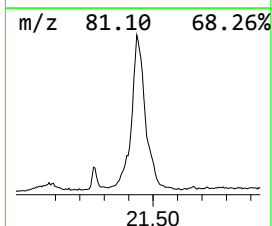
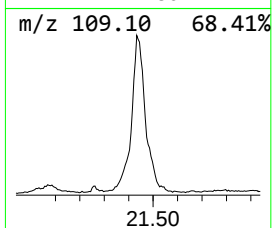
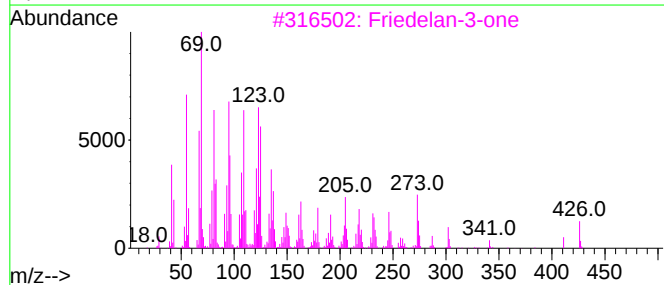
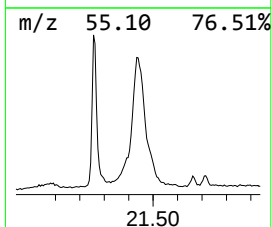
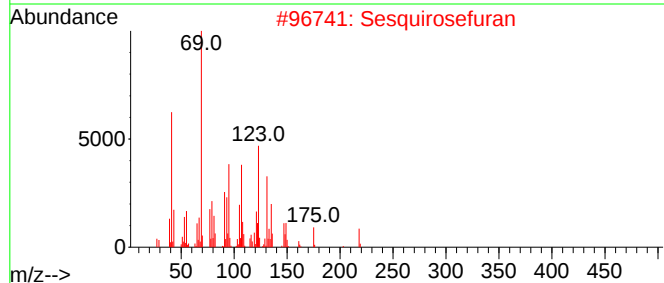
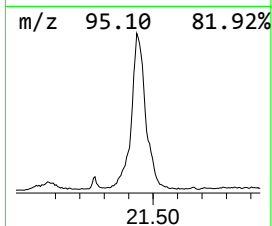
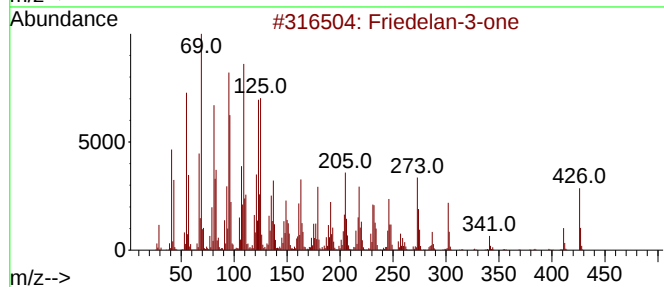
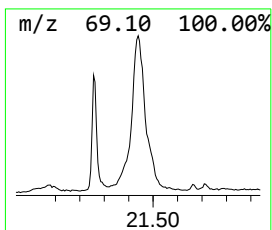
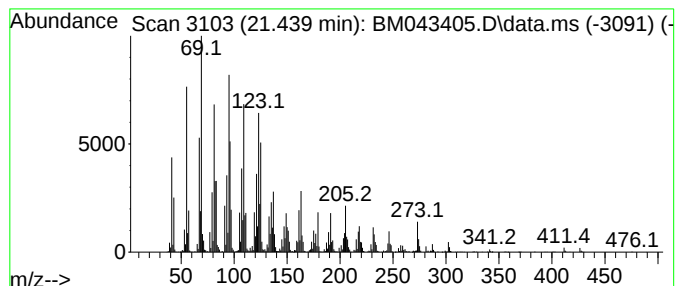
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Sesquirosefuran Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.439	34.92 ng/ul	8064010	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	99
2			Sesquirosefuran	218	C15H22O	039007-93-7	84
3			Friedelan-3-one	426	C30H50O	000559-74-0	64
4			2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	60
5			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043405.D
Acq On : 18 Dec 2023 22:22
Operator : MA/JU
Sample : 05807-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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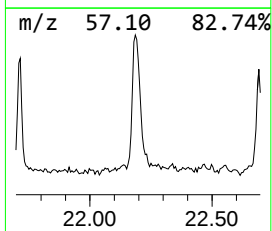
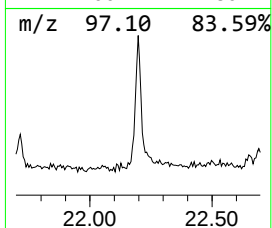
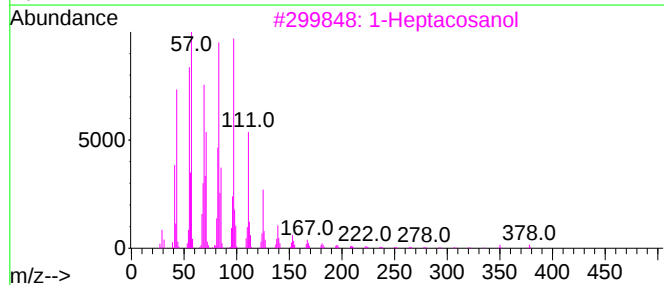
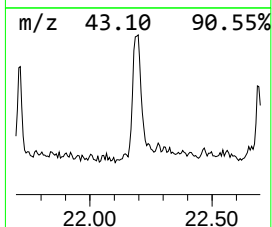
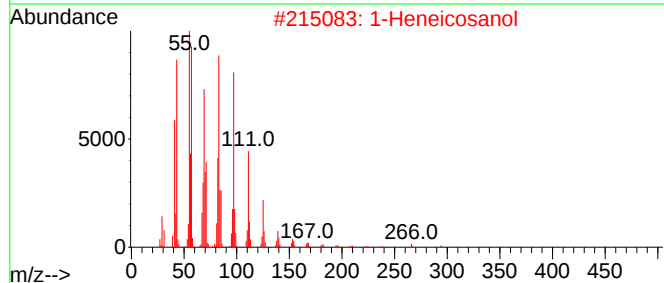
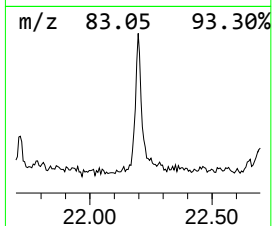
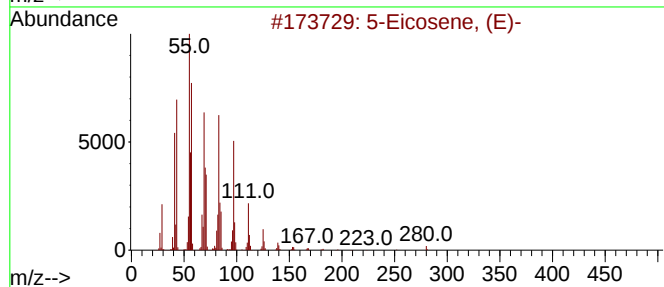
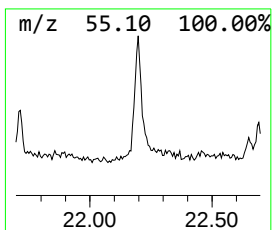
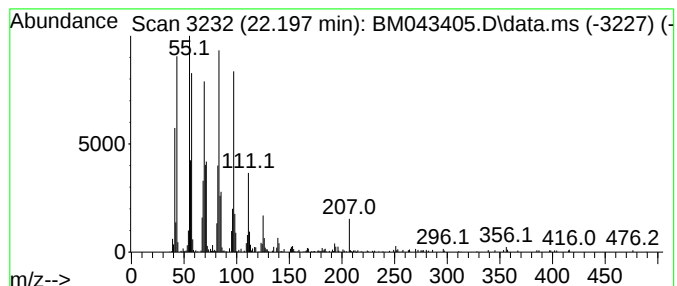
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.197	2.39 ng/ul	55222	Chrysene-d12	21.538

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	1-Heptacosanol		396	C27H56O	002004-39-9	94
4	Behenic alcohol		326	C22H46O	000661-19-8	94
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043405.D
Acq On : 18 Dec 2023 22:22
Operator : MA/JU
Sample : 05807-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.669	2.3	ng/ul	381632	1	7.992	3284770	20.0
Propanoic acid,...	3.710	3.5	ng/ul	583441	1	7.992	3284770	20.0
Butanoic acid	4.298	132.1	ng/ul	21688800	1	7.992	3284770	20.0
n-Hexadecanoic ...	18.268	5.7	ng/ul	1469680	4	17.368	5142590	20.0
Trichloroacetic...	21.256	8.6	ng/ul	1993640	5	21.538	4618200	20.0
Sesquirosefuran	21.439	34.9	ng/ul	8064010	5	21.538	4618200	20.0
(DEL) Alkane: S...	22.197	2.4	ng/ul	552222	5	21.538	4618200	20.0