

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043414.D
 Acq On : 19 Dec 2023 04:23
 Operator : MA/JU
 Sample : 05807-11
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AZ3

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: BM043414.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	43	rVB	159107	207857	0.81%	0.088%
2	3.675	79	83	102	rVB2	135911	271405	1.06%	0.115%
3	3.810	102	106	125	rBV	1736669	2723579	10.60%	1.153%
4	4.181	136	169	172	rBV	1372112	7473045	29.10%	3.163%
5	4.822	273	278	285	rBV	36092	54235	0.21%	0.023%
6	5.069	317	320	330	rVB2	20685	36165	0.14%	0.015%
7	5.287	349	357	374	rVB	11369538	17301138	67.37%	7.322%
8	6.063	482	489	499	rVB2	36974	69588	0.27%	0.029%
9	6.981	637	645	649	rBV	35869	64544	0.25%	0.027%
10	7.151	667	674	686	rBV	2601445	4041435	15.74%	1.710%
11	7.328	695	704	721	rVB	1953569	3121685	12.15%	1.321%
12	7.516	729	736	747	rBV	2374499	3907898	15.22%	1.654%
13	7.875	791	797	805	rVB	263036	412150	1.60%	0.174%
14	7.993	808	817	820	rBV	1703816	3002506	11.69%	1.271%
15	8.028	820	823	837	rVB	2657201	3946925	15.37%	1.670%
16	8.345	871	877	883	rVB	28568	49949	0.19%	0.021%
17	8.704	930	938	952	rBV	2953440	4864368	18.94%	2.059%
18	9.163	1008	1016	1026	rBV	2330693	3824723	14.89%	1.619%
19	9.734	1104	1113	1119	rBV	111632	179025	0.70%	0.076%
20	9.881	1129	1138	1153	rBV	1864740	3195819	12.44%	1.353%
21	10.416	1220	1229	1248	rBV	2762617	4688660	18.26%	1.984%
22	10.698	1266	1277	1281	rBV4	18083	50761	0.20%	0.021%
23	10.798	1287	1294	1303	rBV	2284258	3844700	14.97%	1.627%
24	10.945	1310	1319	1336	rBV	2518108	4331925	16.87%	1.833%
25	11.351	1381	1388	1396	rVB7	27539	66470	0.26%	0.028%
26	11.551	1414	1422	1434	rBV	116671	247440	0.96%	0.105%
27	12.216	1529	1535	1541	rBV	34694	51643	0.20%	0.022%
28	12.381	1558	1563	1569	rBV2	47476	83041	0.32%	0.035%
29	12.969	1657	1663	1668	rBV5	19346	42183	0.16%	0.018%
30	13.445	1736	1744	1748	rBV	52262	89863	0.35%	0.038%
31	13.522	1753	1757	1759	rVV	41608	63392	0.25%	0.027%
32	13.557	1759	1763	1768	rVV	69090	123120	0.48%	0.052%
33	13.904	1816	1822	1828	rBV4	16552	32596	0.13%	0.014%
34	14.039	1837	1845	1853	rBV	4163442	5833322	22.71%	2.469%
35	14.316	1885	1892	1905	rVB	5021277	7584723	29.53%	3.210%
36	14.622	1936	1944	1952	rBV	2935656	4342740	16.91%	1.838%

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
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37	14.822	1971	1978	1996	rBV	2073906	3208820	12.49%	1.358%
38	15.033	2010	2014	2020	rVV4	32135	46122	0.18%	0.020%
39	15.616	2105	2113	2120	rBV	6118739	8599770	33.48%	3.640%
40	15.733	2127	2133	2144	rBV	1778260	2461098	9.58%	1.042%
41	15.851	2149	2153	2162	rVB4	27530	52388	0.20%	0.022%
42	15.945	2164	2169	2174	rVV2	35224	48614	0.19%	0.021%
43	16.069	2185	2190	2200	rVB	34191	60882	0.24%	0.026%
44	16.327	2226	2234	2240	rBV3	32639	53712	0.21%	0.023%
45	16.392	2241	2245	2250	rVB5	28155	44001	0.17%	0.019%
46	16.557	2268	2273	2279	rBV3	46169	66286	0.26%	0.028%
47	16.763	2303	2308	2315	rBV2	80191	127374	0.50%	0.054%
48	17.121	2365	2369	2374	rBV3	20786	41132	0.16%	0.017%
49	17.363	2404	2410	2416	rBV	3065762	4335615	16.88%	1.835%
50	17.410	2416	2418	2421	rVV2	81968	87603	0.34%	0.037%
51	17.463	2421	2427	2436	rVB	5801455	8293396	32.29%	3.510%
52	17.733	2468	2473	2482	rVB8	41377	90476	0.35%	0.038%
53	17.863	2491	2495	2499	rBV2	54398	74376	0.29%	0.031%
54	18.268	2558	2564	2581	rBV	933020	1594943	6.21%	0.675%
55	18.557	2610	2613	2616	rBV	33672	40097	0.16%	0.017%
56	18.592	2616	2619	2627	rVB9	29938	51089	0.20%	0.022%
57	18.692	2633	2636	2641	rVB2	31950	42150	0.16%	0.018%
58	18.845	2659	2662	2666	rVB5	27028	33289	0.13%	0.014%
59	18.927	2671	2676	2680	rBV4	83748	108338	0.42%	0.046%
60	19.121	2705	2709	2713	rBV5	49106	72961	0.28%	0.031%
61	19.192	2717	2721	2725	rVB	122721	145532	0.57%	0.062%
62	19.245	2726	2730	2735	rBV	44992	51004	0.20%	0.022%
63	19.315	2738	2742	2749	rVB2	67311	90477	0.35%	0.038%
64	19.392	2750	2755	2757	rBV3	124088	180221	0.70%	0.076%
65	19.539	2775	2780	2790	rBV	374123	621321	2.42%	0.263%
66	19.751	2809	2816	2823	rBV	6516577	8434759	32.84%	3.570%
67	19.804	2823	2825	2829	rVB2	37260	42983	0.17%	0.018%
68	19.974	2850	2854	2858	rVB5	91882	117286	0.46%	0.050%
69	20.268	2900	2904	2907	rBV	215216	286692	1.12%	0.121%
70	20.304	2907	2910	2916	rVV	370716	430051	1.67%	0.182%
71	20.368	2918	2921	2926	rVB	69150	81857	0.32%	0.035%
72	20.621	2960	2964	2969	rBV3	189894	321798	1.25%	0.136%
73	20.798	2989	2994	2998	rVB	192087	270097	1.05%	0.114%
74	20.951	3017	3020	3025	rBV6	67236	95059	0.37%	0.040%
75	21.256	3068	3072	3081	rBV	2812606	3885733	15.13%	1.645%
76	21.339	3082	3086	3091	rVB2	332468	426228	1.66%	0.180%

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77	21.392	3091	3095	3100	rBV	255976	318352	1.24%	0.135%
78	21.451	3100	3105	3110	rBV	876011	1070164	4.17%	0.453%
79	21.498	3110	3113	3115	rBV2	123675	147371	0.57%	0.062%
80	21.539	3115	3120	3136	rVB	3135839	4346844	16.93%	1.840%
81	21.662	3139	3141	3144	rVV3	81114	77824	0.30%	0.033%
82	21.709	3146	3149	3154	rVB	283935	381700	1.49%	0.162%
83	22.198	3225	3232	3242	rBV2	1531156	3139785	12.23%	1.329%
84	22.280	3243	3246	3252	rVB	276774	361647	1.41%	0.153%
85	22.686	3312	3315	3320	rVB2	277849	425791	1.66%	0.180%
86	23.256	3407	3412	3417	rBV	1912625	3211416	12.50%	1.359%
87	23.303	3417	3420	3432	rVB	666459	1198165	4.67%	0.507%
88	23.809	3498	3506	3515	rBV2	4286722	8335795	32.46%	3.528%
89	23.897	3518	3521	3525	rVV3	262253	480345	1.87%	0.203%
90	23.962	3526	3532	3546	rVB	2082285	4285668	16.69%	1.814%
91	24.497	3618	3623	3632	rVB	350580	748139	2.91%	0.317%
92	24.650	3643	3649	3656	rVB	832401	1786189	6.95%	0.756%
93	24.744	3659	3665	3676	rVV2	674057	1604589	6.25%	0.679%
94	24.874	3681	3687	3698	rVB	873674	2181221	8.49%	0.923%
95	26.350	3931	3938	3947	rVB2	518595	1370486	5.34%	0.580%
96	26.715	3992	4000	4015	rVB5	729255	2528754	9.85%	1.070%
97	27.656	4149	4160	4174	rVB2	4037080	13707560	53.37%	5.801%
98	28.097	4222	4235	4260	rVB2	3273985	13241541	51.56%	5.604%
99	28.497	4293	4303	4321	rVB3	2595554	10314381	40.16%	4.365%
100	28.926	4363	4376	4400	rVB2	6027596	25682540	100.00%	10.869%

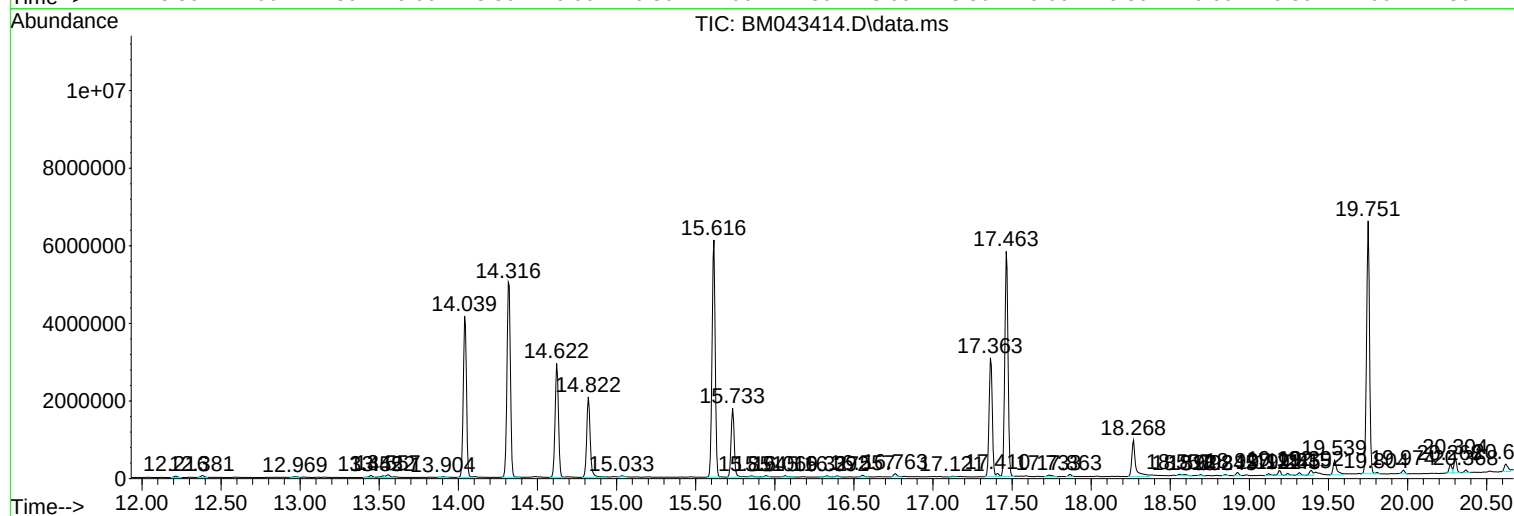
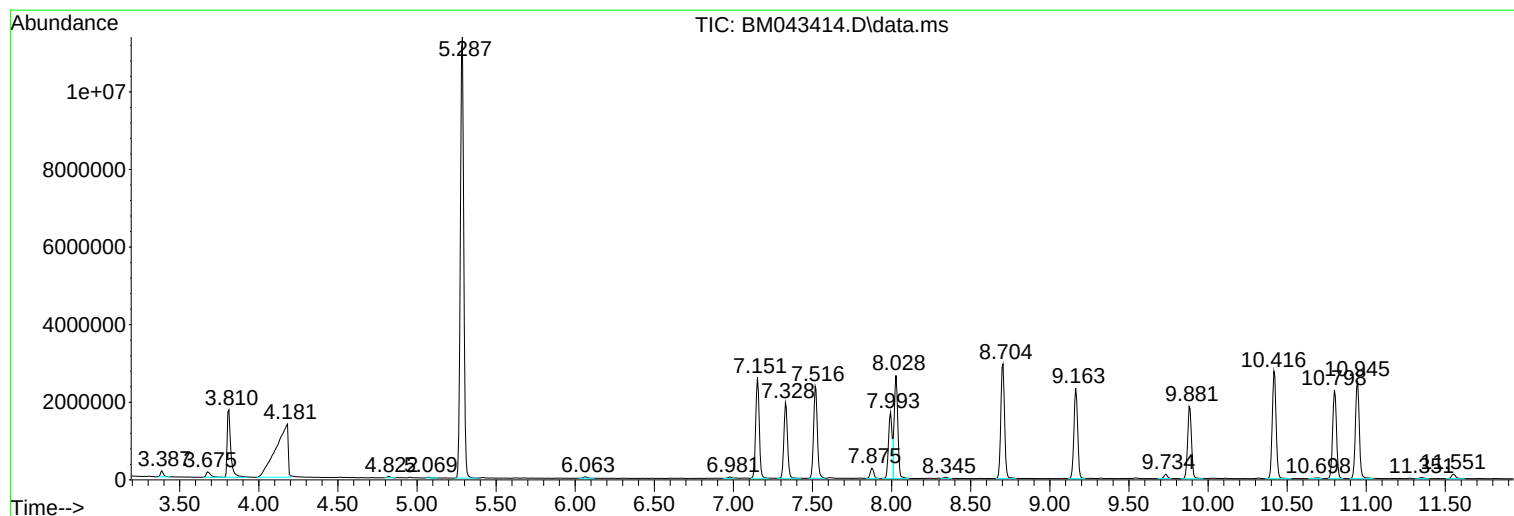
Sum of corrected areas: 236286515

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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



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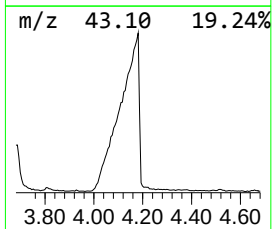
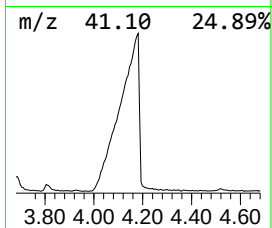
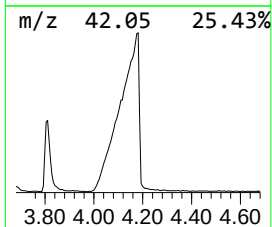
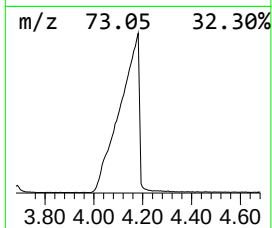
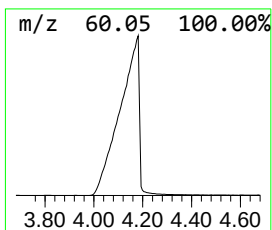
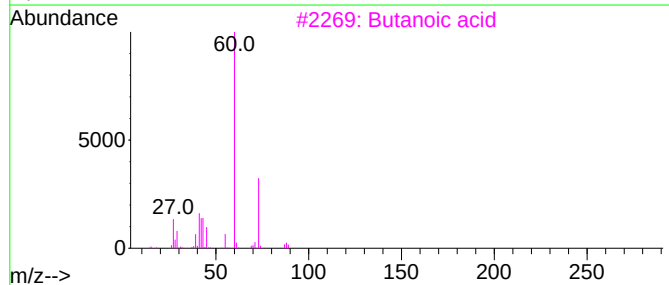
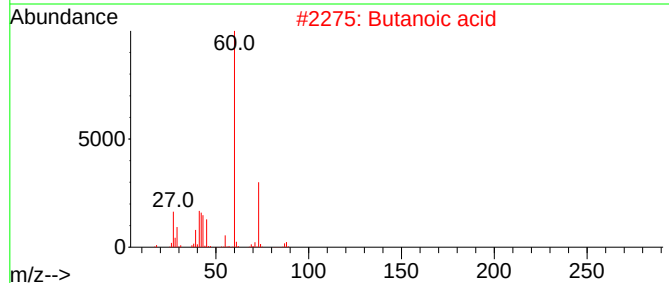
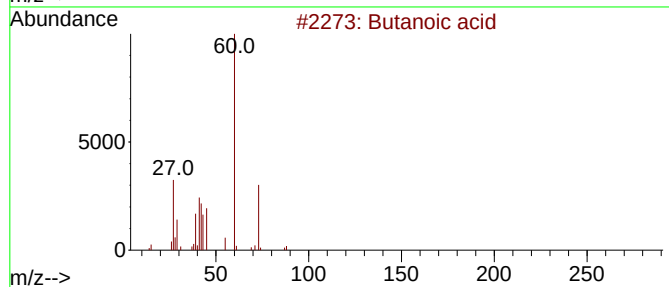
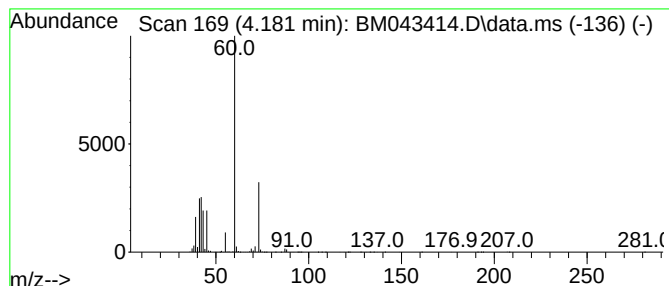
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Butanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.181	49.78 ng/ul	7473050	1,4-Dichlorobenzene-d4	7.993

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	86
2			Butanoic acid	88	C4H8O2	000107-92-6	80
3			Butanoic acid	88	C4H8O2	000107-92-6	80
4			Butanoic acid	88	C4H8O2	000107-92-6	74
5			Pentanoic acid	102	C5H10O2	000109-52-4	50



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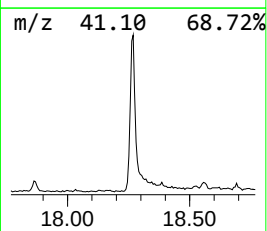
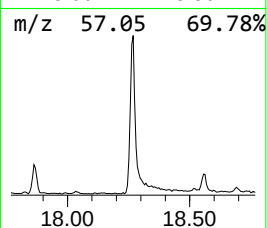
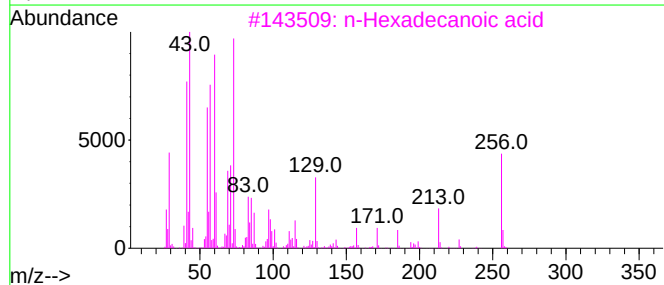
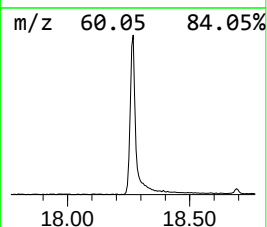
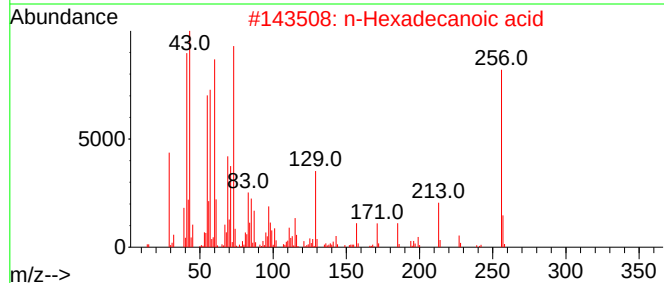
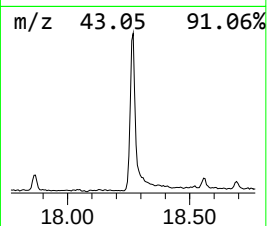
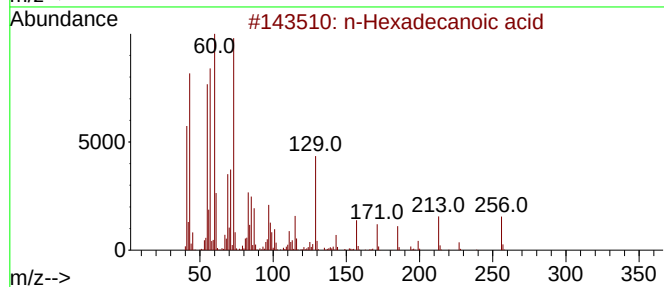
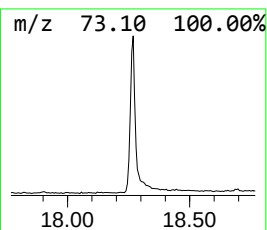
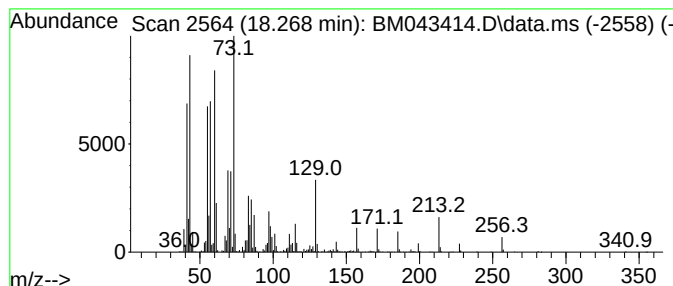
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	7.36 ng/ul	1594940	Phenanthrene-d10	17.363

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	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	93



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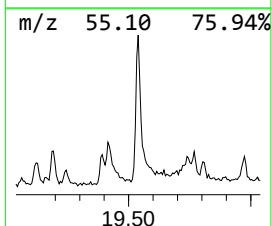
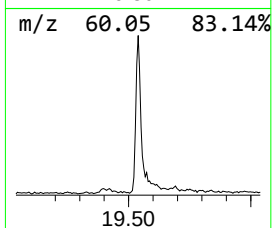
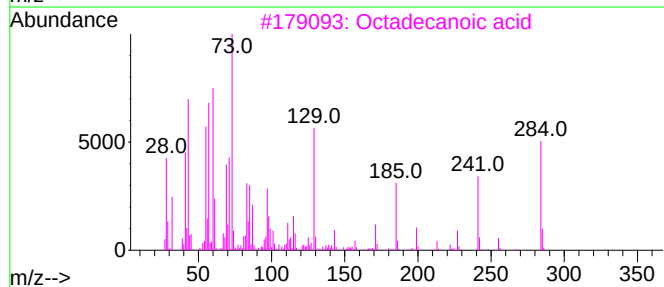
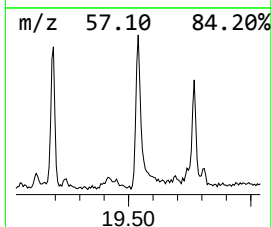
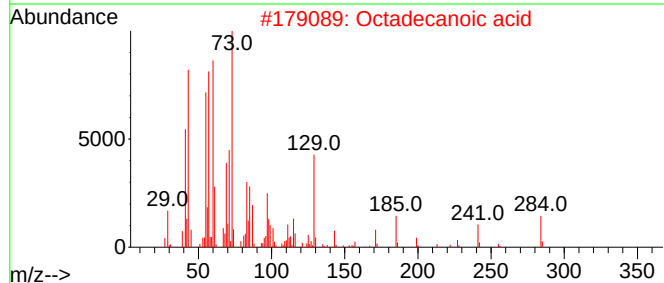
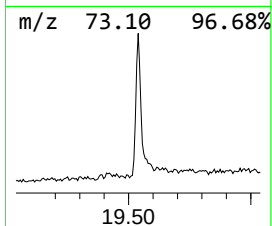
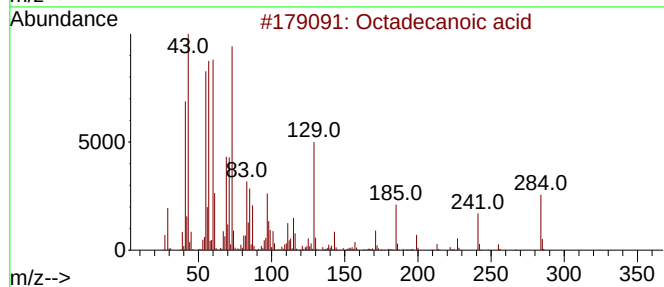
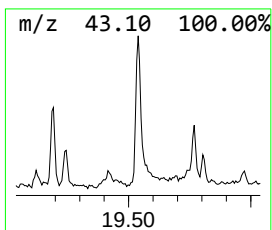
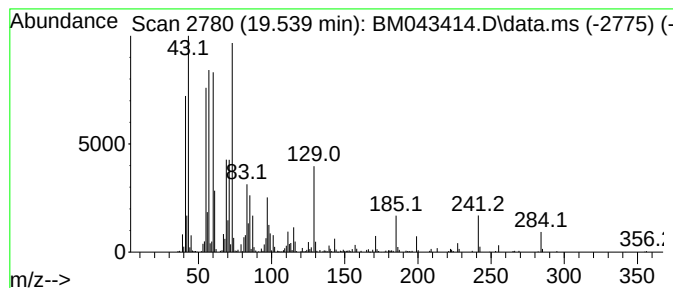
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.539	2.86 ng/ul	621321	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	97
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Octadecanoic acid	284	C18H36O2	000057-11-4	95



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Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
Operator : MA/JU
Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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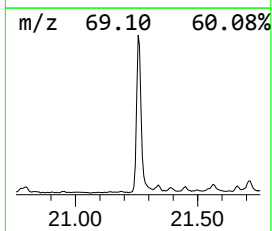
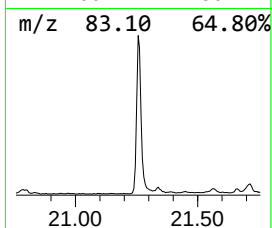
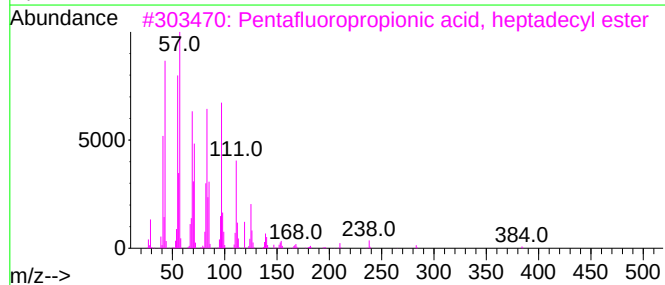
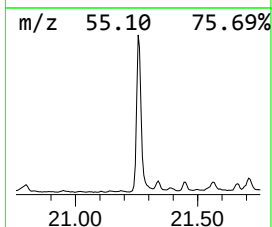
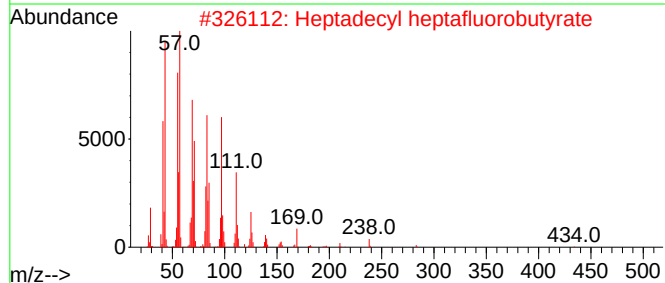
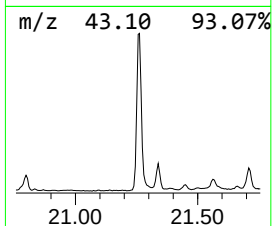
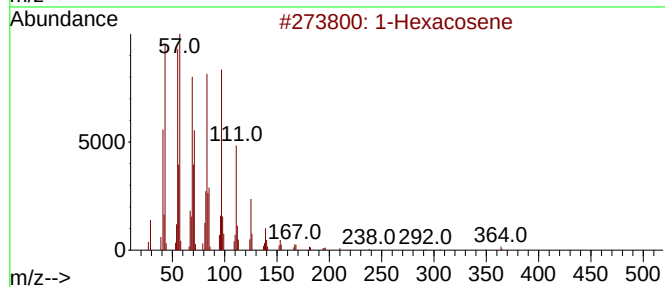
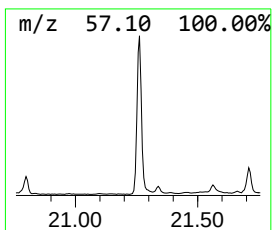
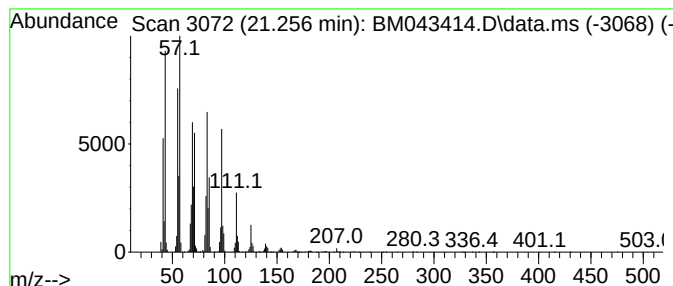
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.256	17.88 ng/ul	3885730	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	91
3	Pentafluoropropionic acid, hepta...			402	C20H35F5O2	959218-78-1	91
4	Nonadecyl pentafluoropropionate			430	C22H39F5O2	1000351-88-8	91
5	Pentafluoropropionic acid, octad...			416	C21H37F5O2	959261-25-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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Sample : 05807-11
Misc :
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Instrument :
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ClientSampleId :
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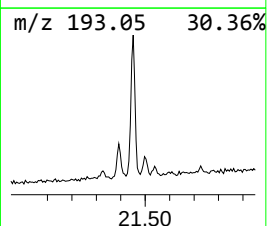
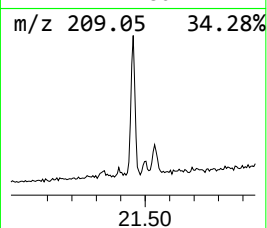
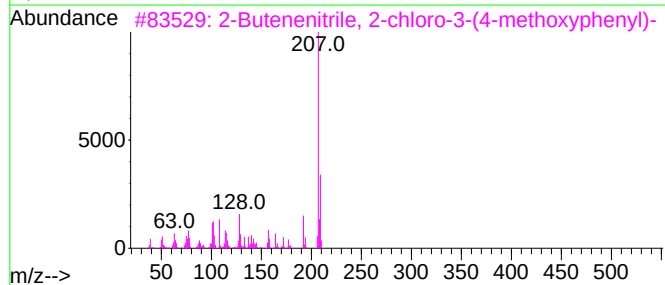
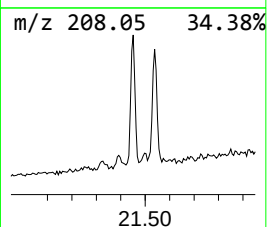
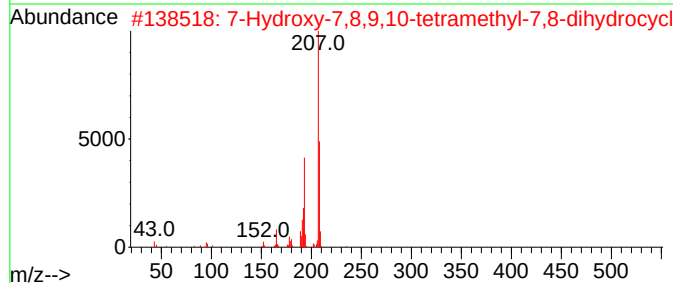
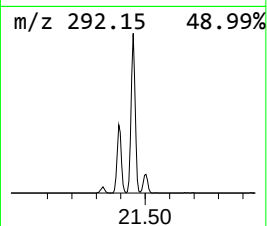
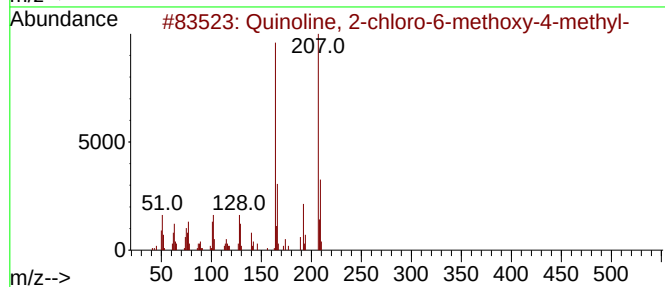
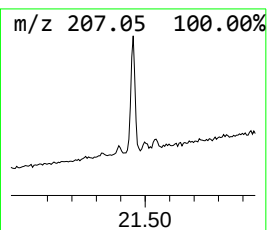
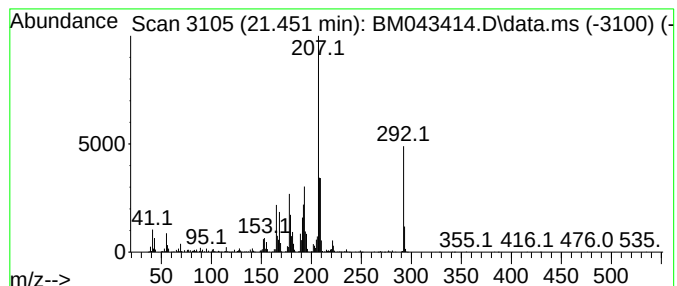
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-01 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.451	4.92 ng/ul	1070160	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 2-chloro-6-methoxy-4-...	207	C11H10ClNO	006340-55-2	43		
2	7-Hydroxy-7,8,9,10-tetramethyl-7...	252	C18H20O	1000110-34-9	43		
3	2-Butenenitrile, 2-chloro-3-(4-m...	207	C11H10ClNO	1010305-66-7	38		
4	Benzene, 1-ethoxy-4-[(4-pentylph...	292	C21H24O	095480-29-8	38		
5	Quinoline, 4-chloro-6-methoxy-2-...	207	C11H10ClNO	050593-73-2	37		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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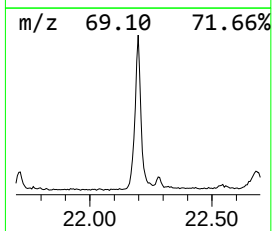
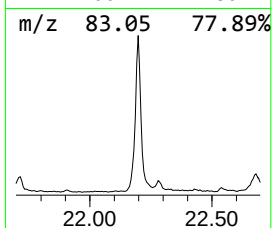
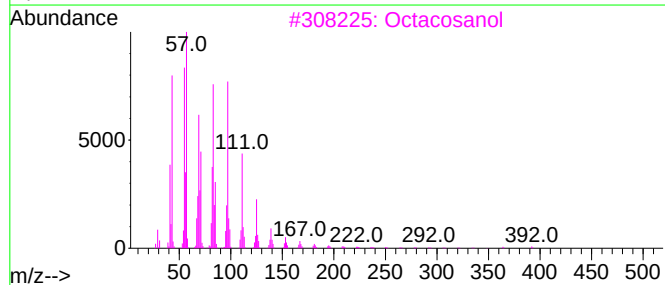
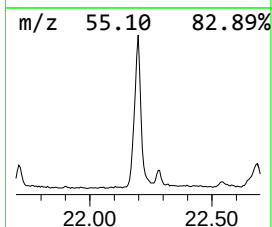
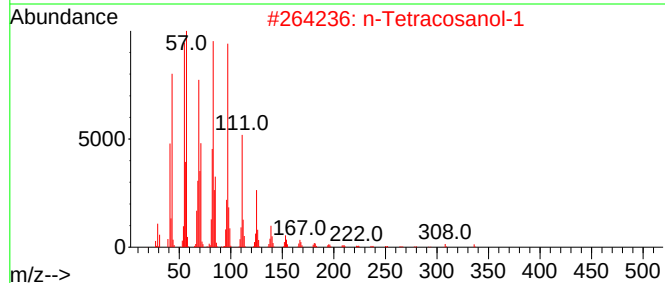
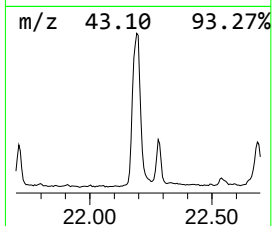
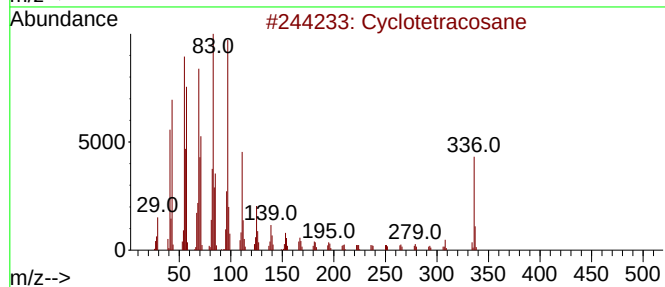
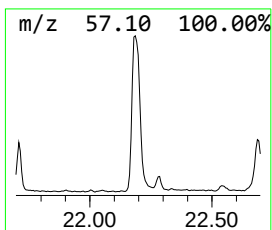
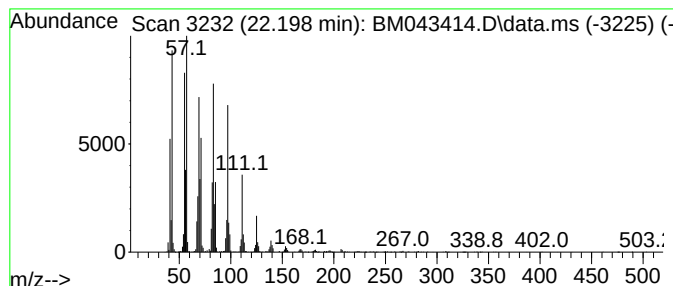
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Cyclic22.198 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.198	14.45 ng/ul	3139790	Chrysene-d12	21.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Octacosanol	410	C28H58O	000557-61-9	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Cyclopentadecane	210	C15H30	000295-48-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

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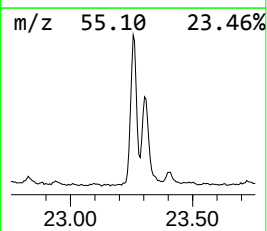
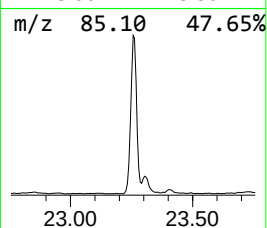
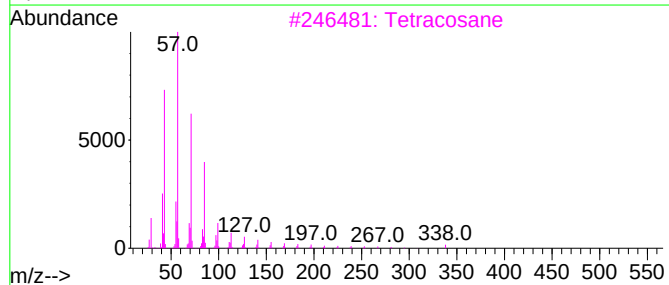
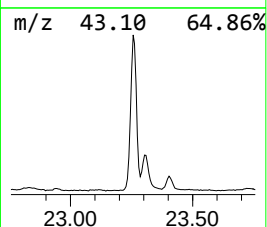
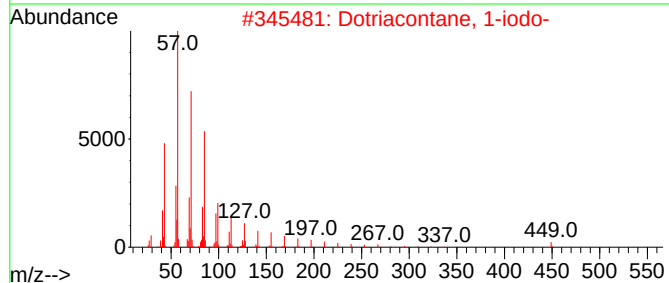
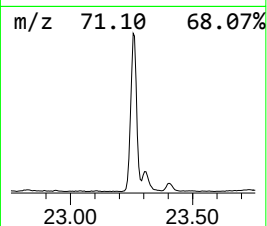
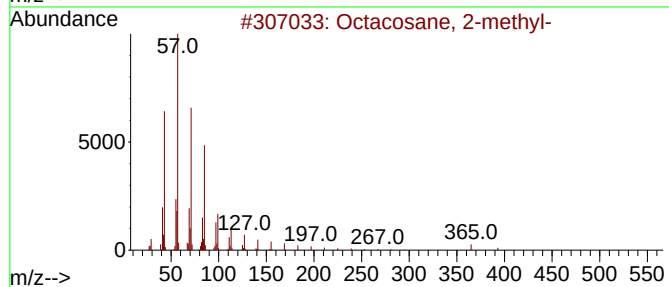
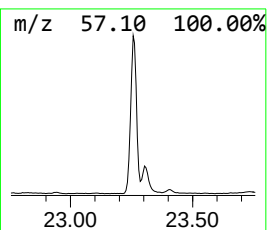
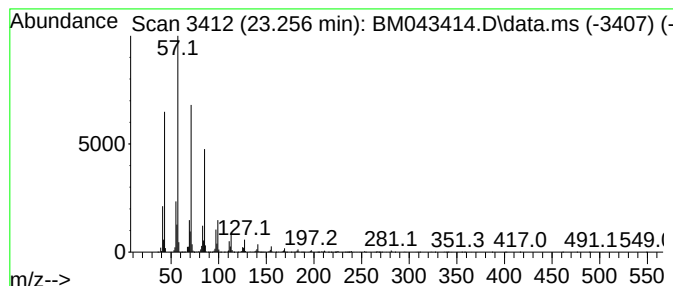
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.256	14.99 ng/ul	3211420	Perylene-d12	23.962

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
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Sample : 05807-11
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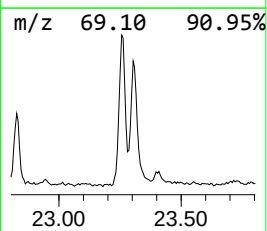
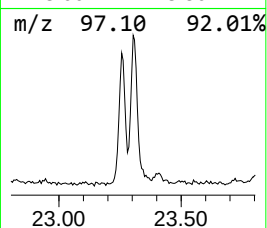
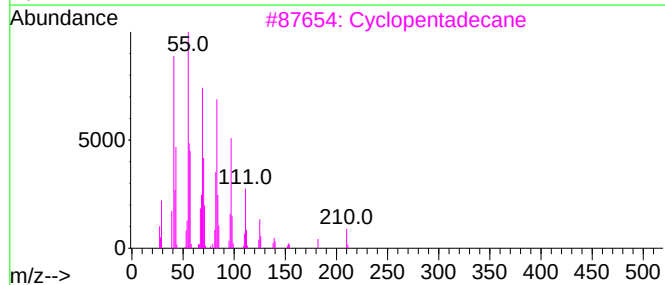
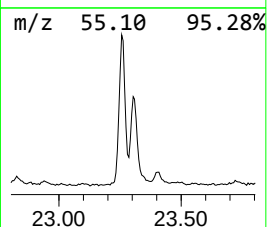
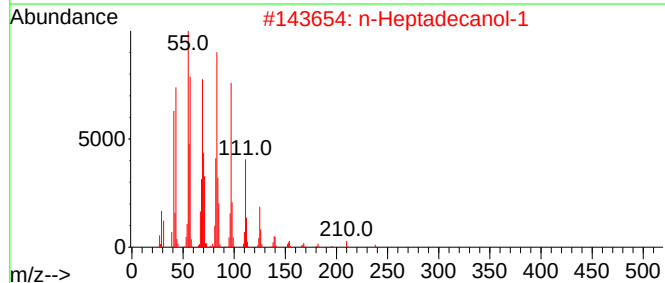
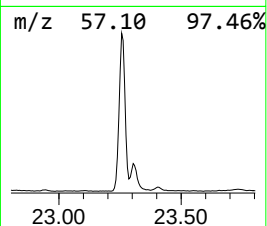
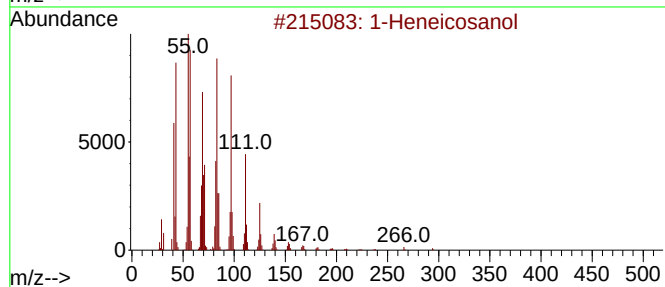
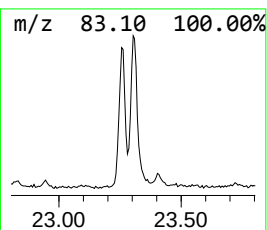
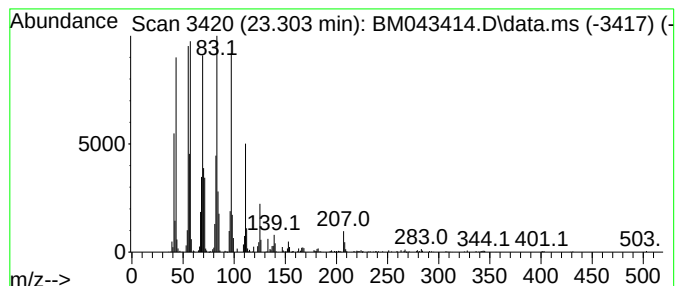
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.303	5.59 ng/ul	1198170	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	Cyclopentadecane	210	C15H30	000295-48-7	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Nonadecene	266	C19H38	018435-45-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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Sample : 05807-11
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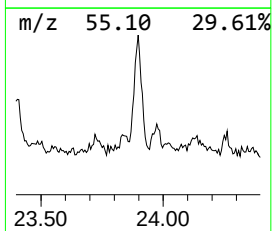
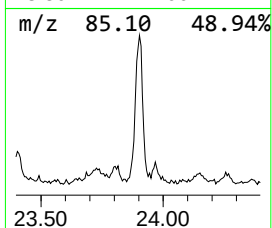
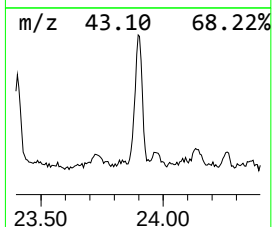
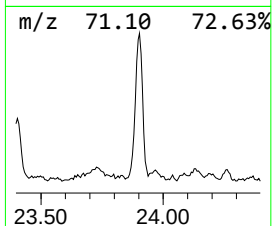
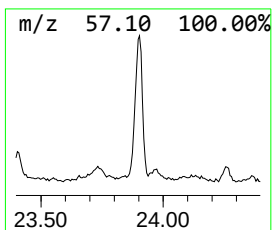
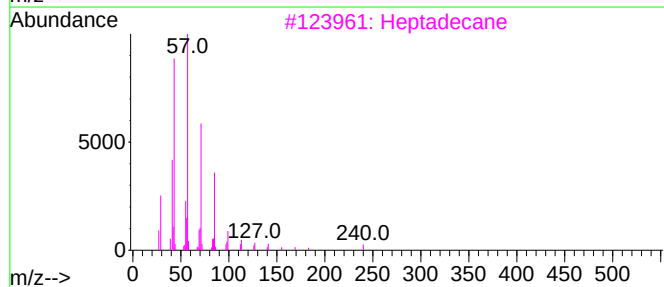
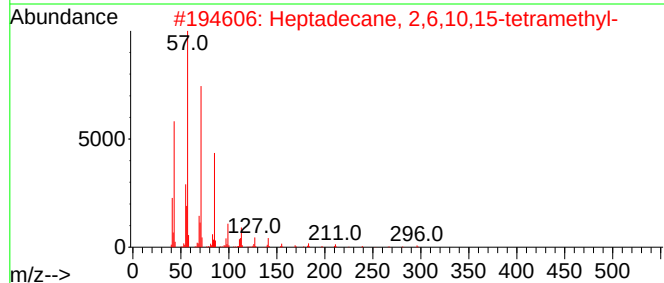
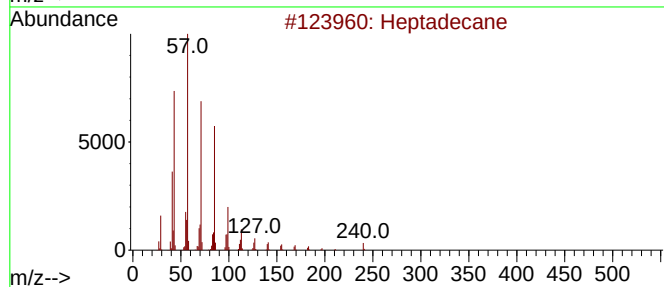
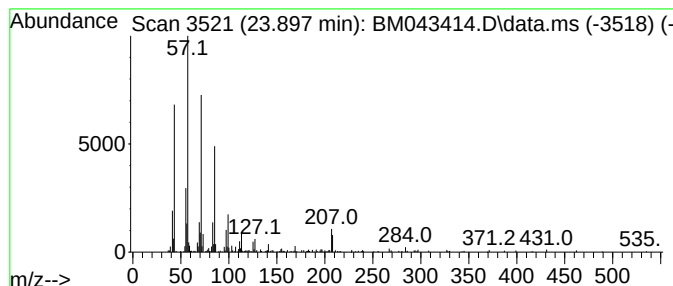
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 (DEL) Alkane: Straight-Chai... Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.897	2.24 ng/ul	480345	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	83
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
3	Heptadecane	240	C17H36	000629-78-7	81
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	80
5	Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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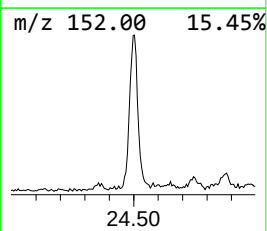
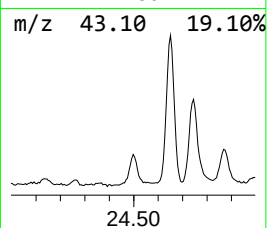
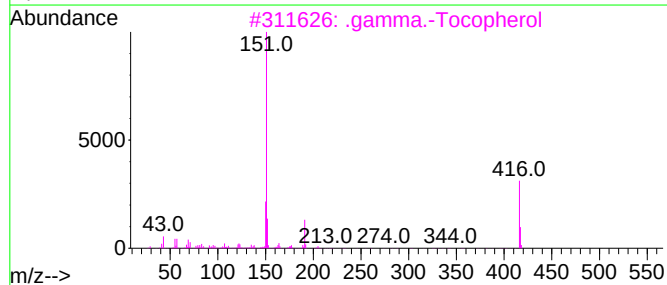
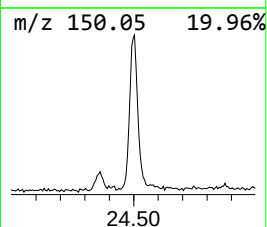
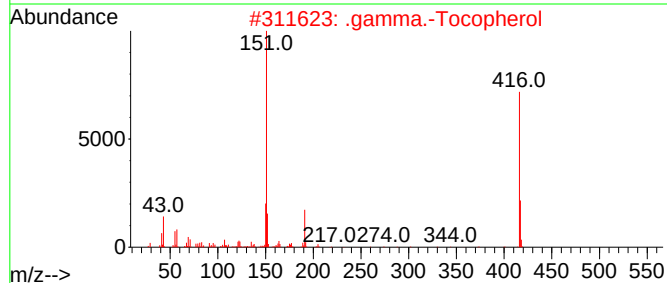
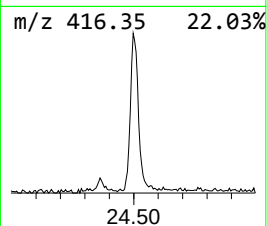
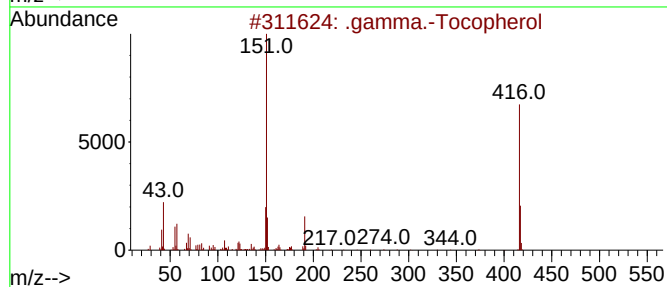
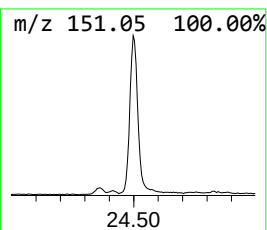
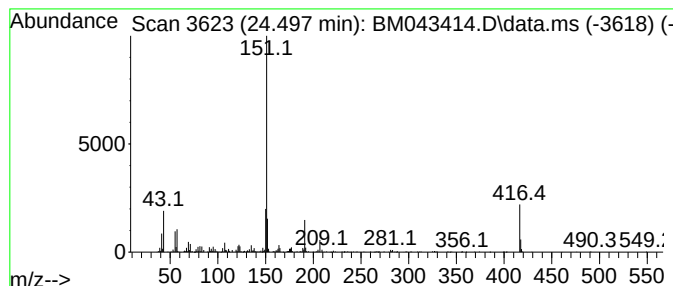
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 .gamma.-Tocopherol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.497	3.49 ng/ul	748139	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	gamma.-Tocopherol	416	C28H48O2	007616-22-0	99	
2	.	gamma.-Tocopherol	416	C28H48O2	007616-22-0	98	
3	.	gamma.-Tocopherol	416	C28H48O2	007616-22-0	97	
4	.	gamma.-Tocopherol	416	C28H48O2	007616-22-0	90	
5		Benzenepropanenitrile, 3,4-dimet...	191	C11H13NO2	049621-56-9	53	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
Operator : MA/JU
Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

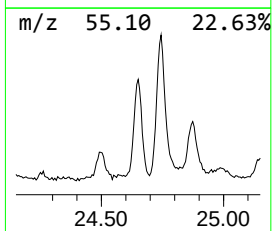
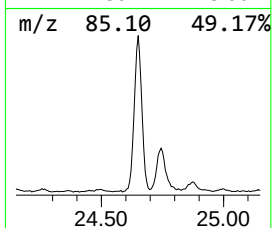
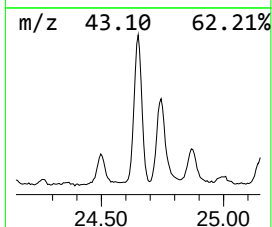
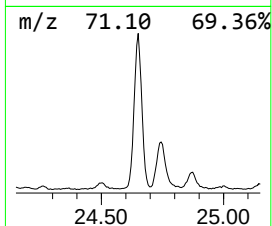
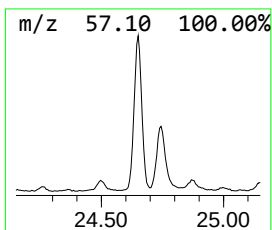
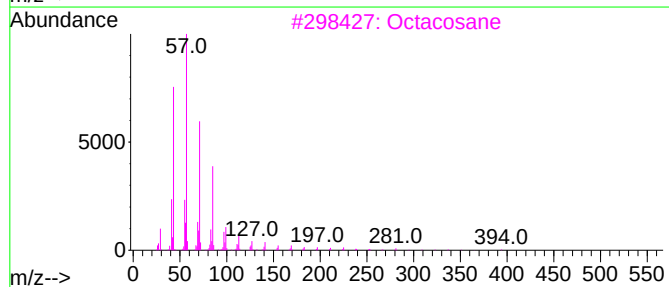
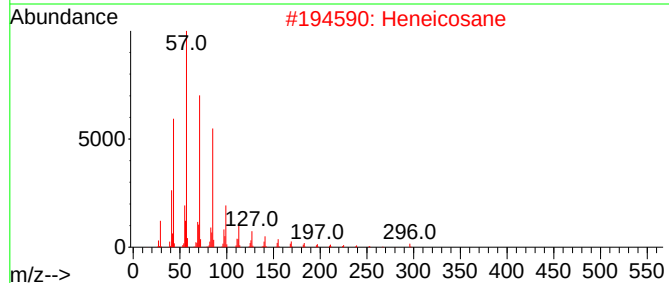
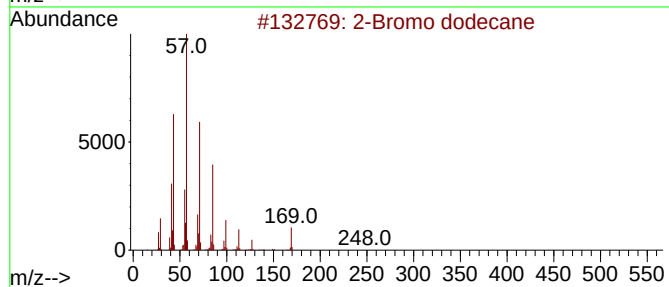
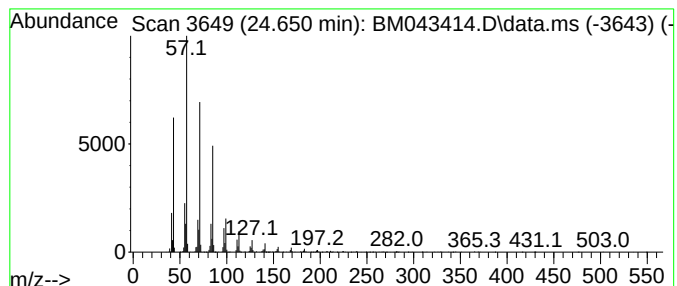
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 13 2-Bromo dodecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.650	8.34 ng/ul	1786190	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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Sample : 05807-11
Misc :
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ClientSampleId :
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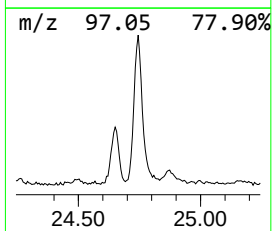
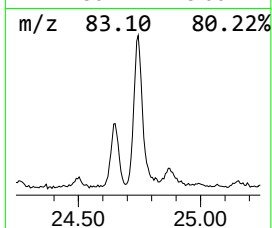
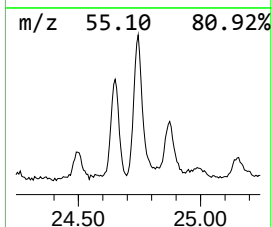
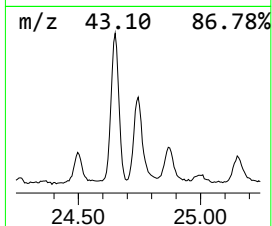
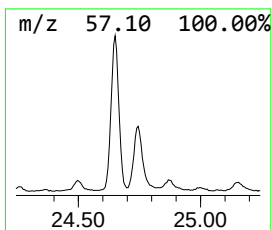
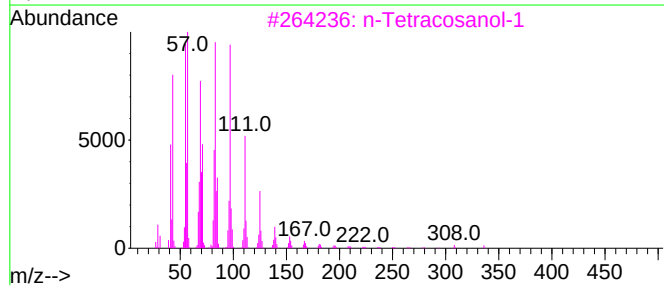
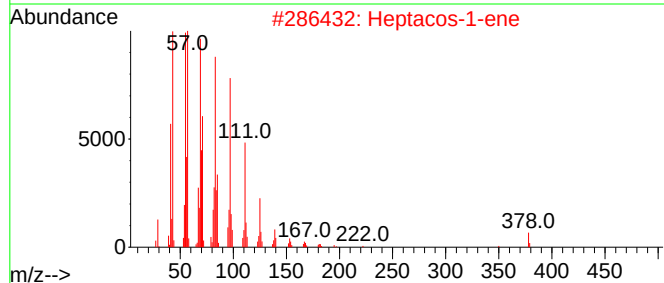
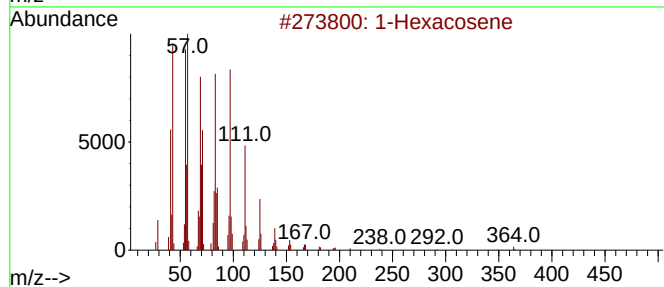
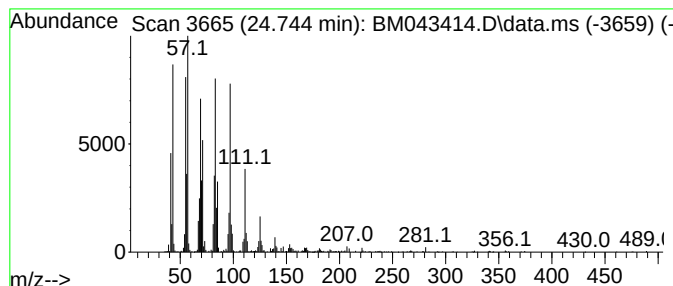
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Quant Title : SVOA CALIBRATION

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

Peak Number 14 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.744	7.49 ng/ul	1604590	Perylene-d12	23.962

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52	018835-33-1	94
2	Heptacos-1-ene		378	C27H54	015306-27-1	94
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
4	Octacosanol		410	C28H58O	000557-61-9	93
5	1-Docosene		308	C22H44	001599-67-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
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Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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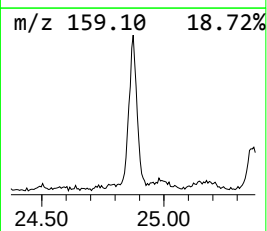
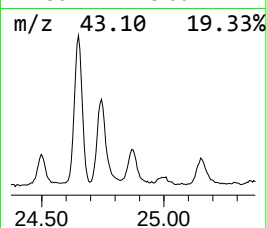
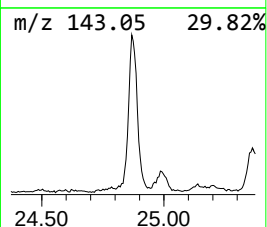
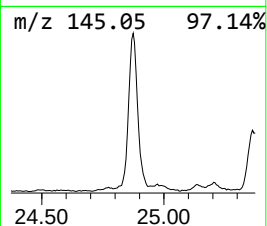
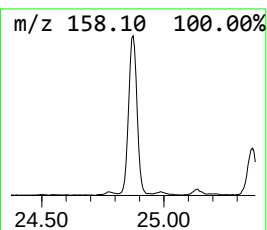
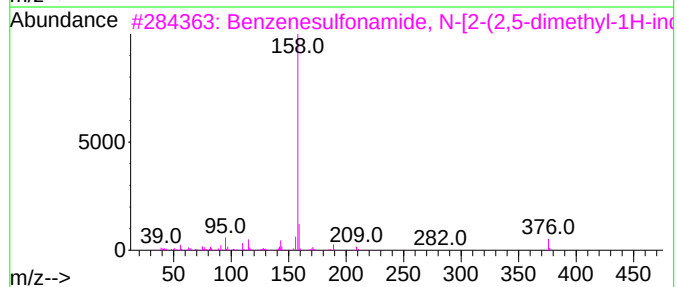
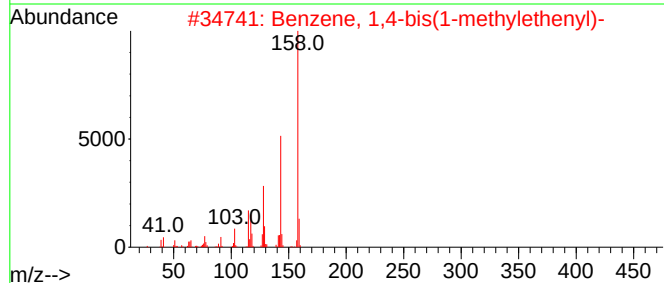
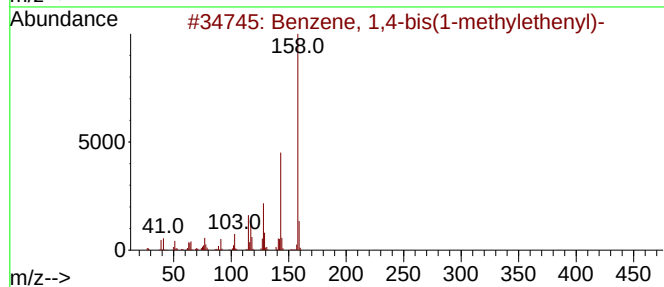
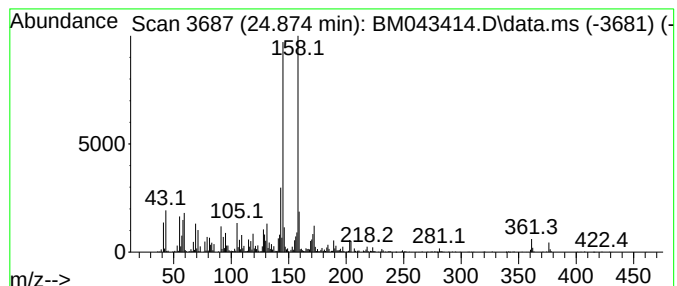
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Quant Title : SVOA CALIBRATION

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

Peak Number 15 Benzene, 1,4-bis(1-methylet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.874	10.18 ng/ul	2181220	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	50
2			Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	43
3			Benzenesulfonamide, N-[2-(2,5-di...	376	C19H21FN2O3S	1000304-39-3	38
4			1H-Indole, 2,3-dihydro-1,3,3-tri...	173	C12H15N	000118-12-7	38
5			1,2,3,4,5,6-Hexahydro-6-methylaz...	200	C13H16N2	015923-78-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
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Acq On : 19 Dec 2023 04:23
Operator : MA/JU
Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

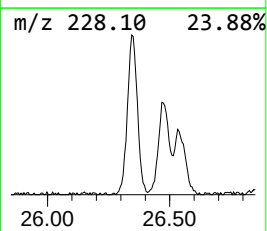
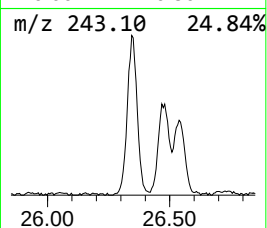
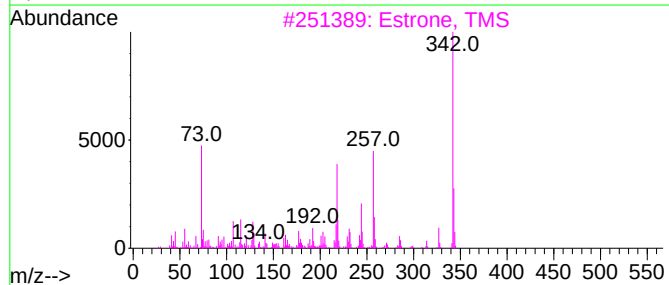
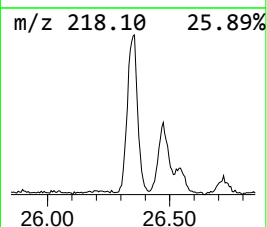
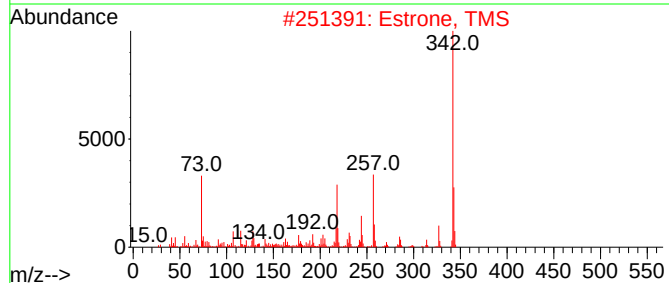
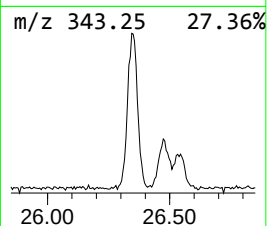
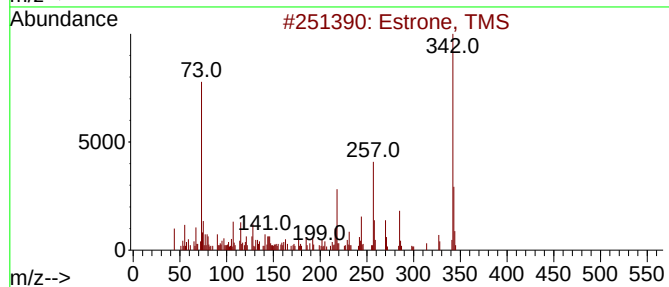
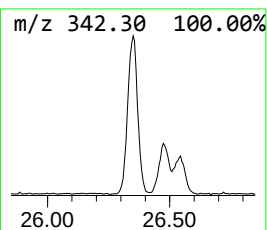
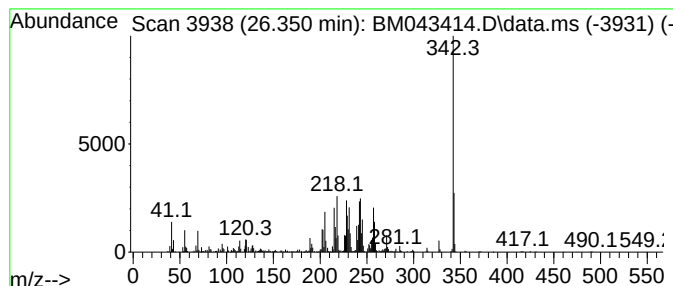
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 16 unknown-02 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.350	6.40 ng/ul	1370490	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estrone, TMS	342	C21H30O2Si	001839-54-9	49
2	Estrone, TMS	342	C21H30O2Si	001839-54-9	38
3	Estrone, TMS	342	C21H30O2Si	001839-54-9	38
4	16-Estrone, TMS derivative	342	C21H30O2Si	077883-20-6	38
5	14-Methyl-11-propyl-3,10,12,14-t...	342	C21H18N4O	1000436-14-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
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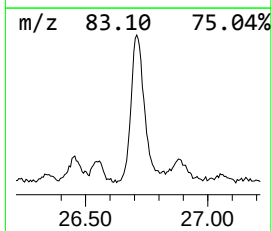
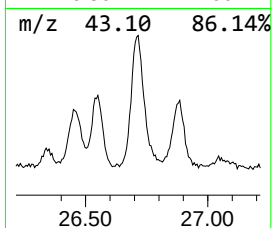
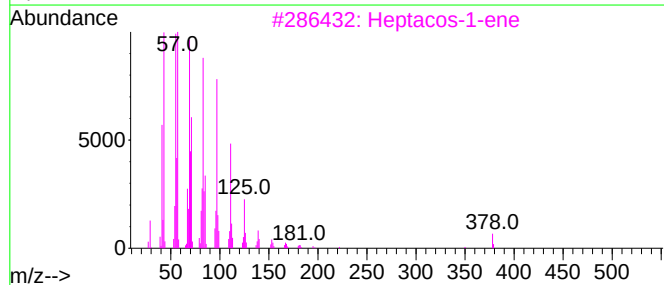
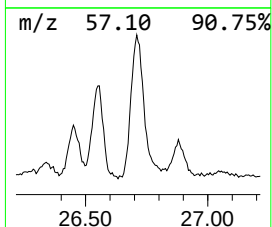
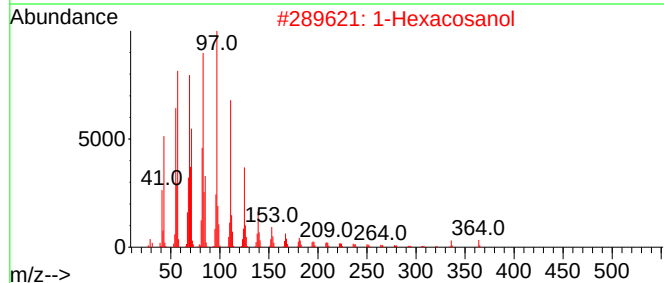
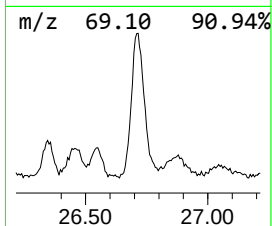
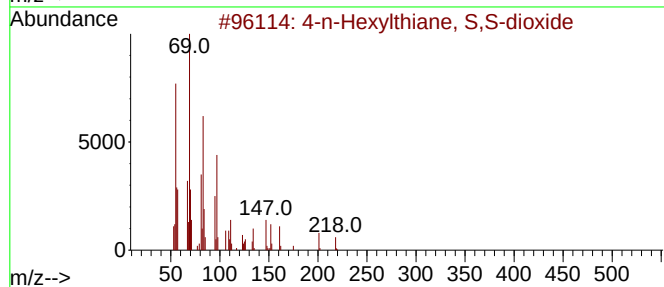
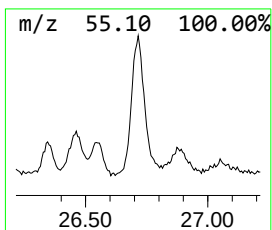
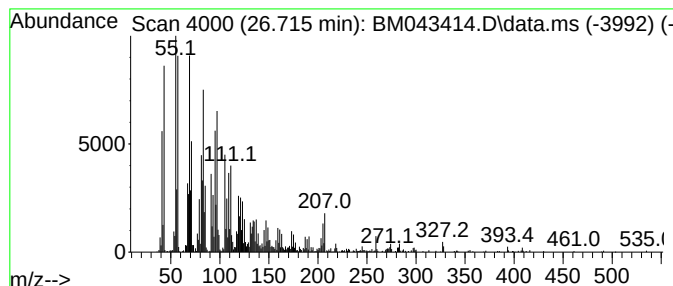
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Quant Title : SVOA CALIBRATION

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

Peak Number 17 4-n-Hexylthiane, S,S-dioxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.715	11.80 ng/ul	2528750	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	78
2	1-Hexacosanol	382	C26H54O	000506-52-5	64
3	Heptacos-1-ene	378	C27H54	015306-27-1	64
4	Octacosanol	410	C28H58O	000557-61-9	64
5	5-Methoxy-10,10-dimethyl-6-methy...	236	C15H24O2	1000511-71-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
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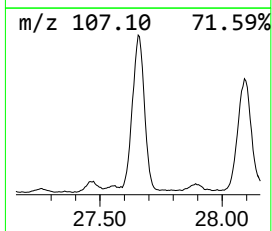
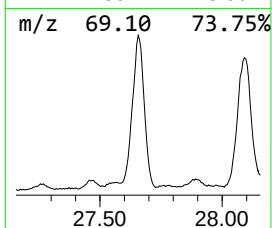
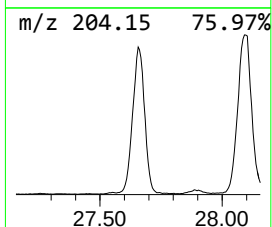
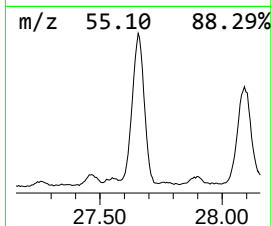
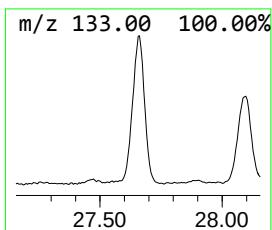
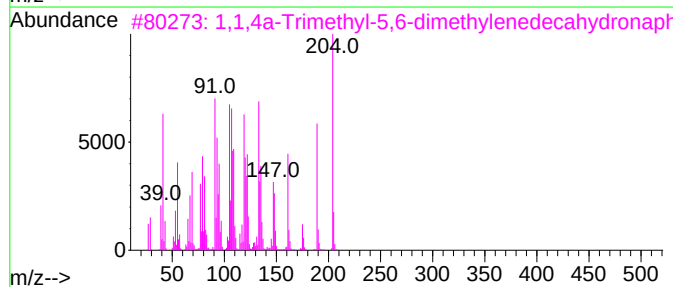
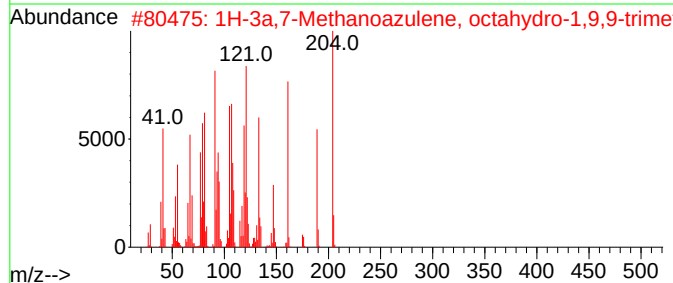
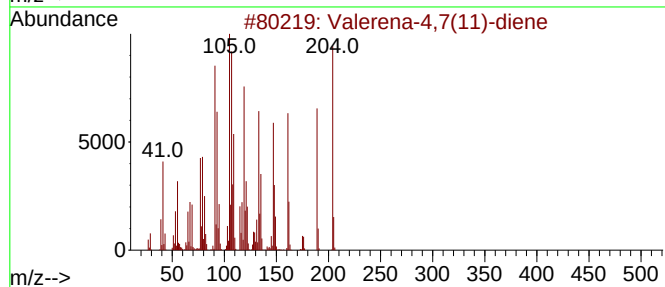
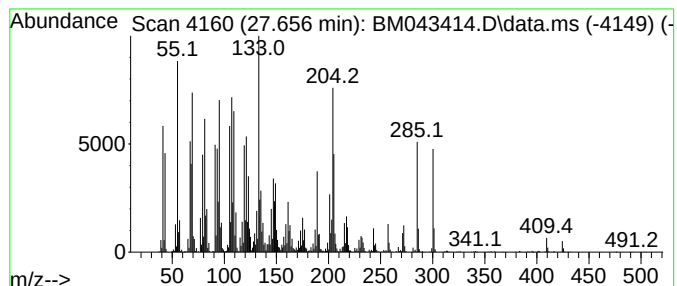
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Quant Title : SVOA CALIBRATION

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

Peak Number 18 Valerena-4,7(11)-diene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
27.656	63.97 ng/ul	13707600	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valerena-4,7(11)-diene	204	C15H24	351222-66-7	58
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	35
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	35
4	Aromandendrene	204	C15H24	000489-39-4	30
5	3-Aminophenol, N,O-bis(trifluoro...	301	C10H5F6NO3	959257-40-0	30



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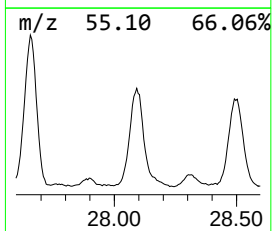
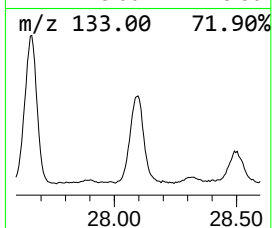
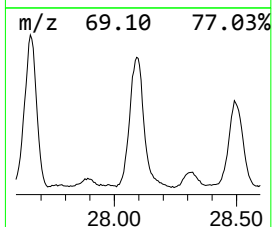
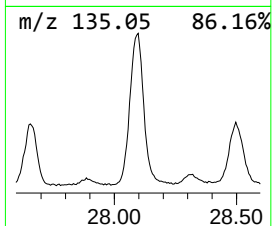
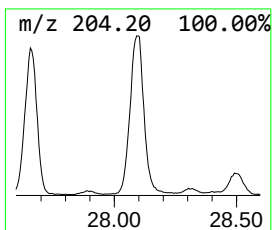
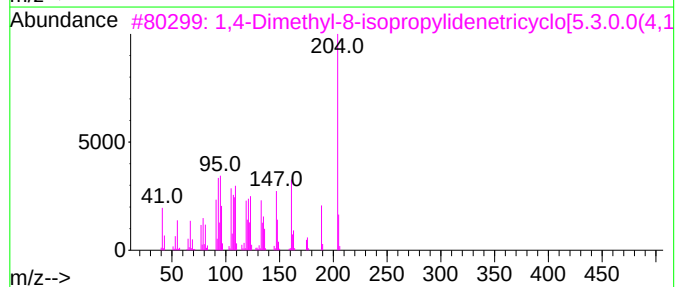
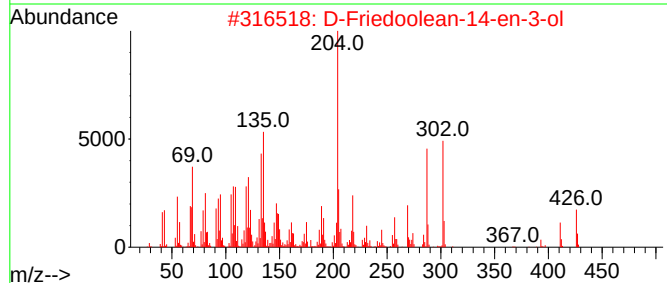
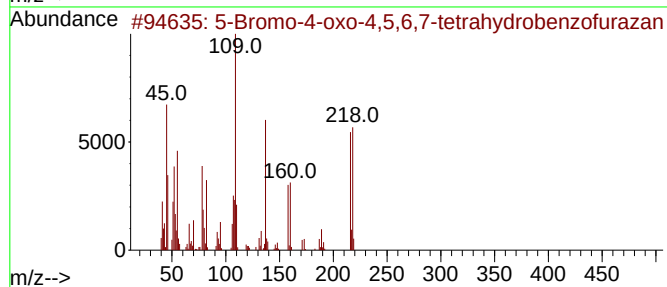
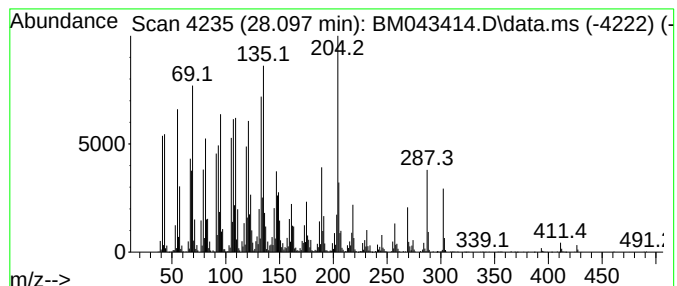
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 19 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.097	61.79 ng/ul	13241500	Perylene-d12	23.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	91
2	D-Friedoolean-14-en-3-ol	426	C30H50O	081654-73-1	87
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	68
4	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	64
5	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
Operator : MA/JU
Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ3

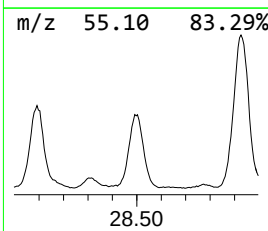
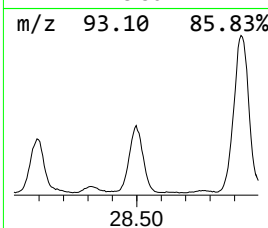
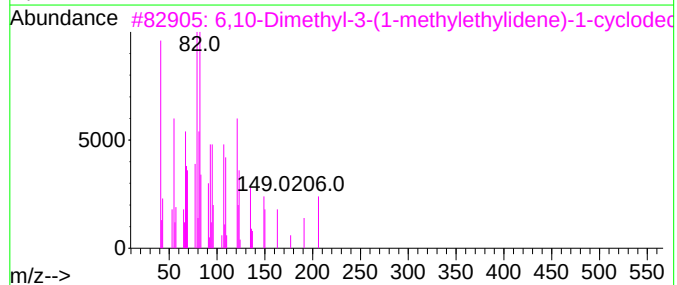
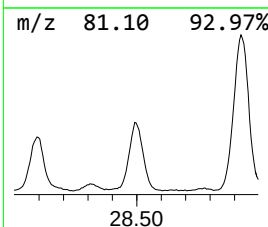
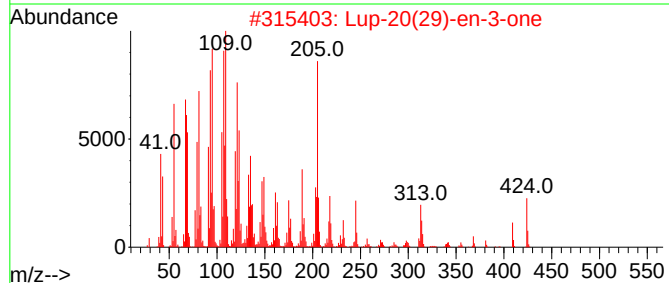
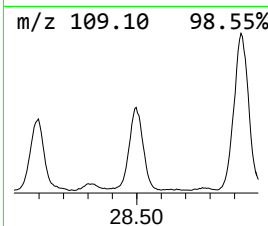
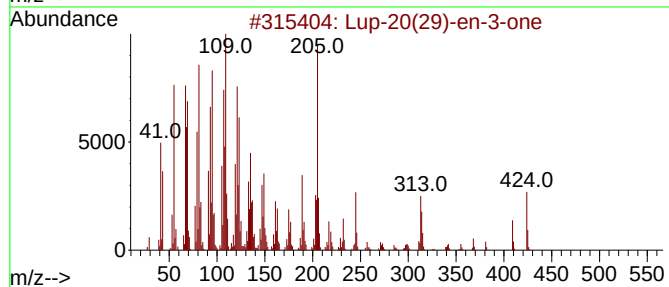
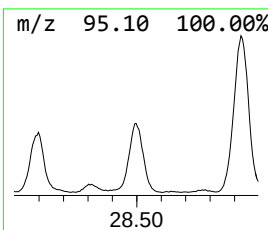
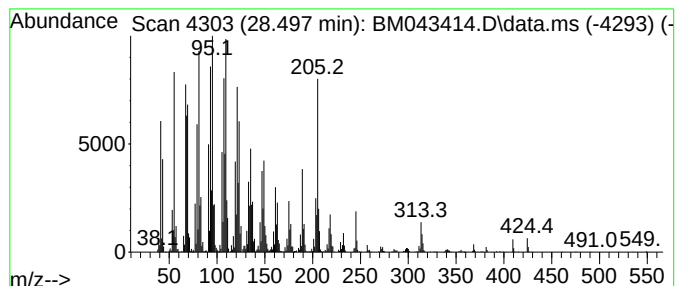
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Quant Title : SVOA CALIBRATION

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

Peak Number 20 Lup-20(29)-en-3-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.497	48.13 ng/ul	10314400	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
3			6,10-Dimethyl-3-(1-methylethylidene)-1-cyclodec	206	C15H26	069239-71-0	83
4			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	83
5			1-Isopropenyl-3-propenylcyclopent-1-en-3-one	150	C11H18	1000192-81-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043414.D
Acq On : 19 Dec 2023 04:23
Operator : MA/JU
Sample : 05807-11
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ3

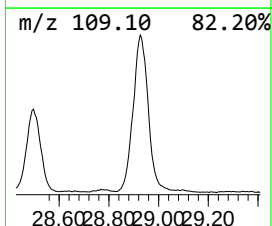
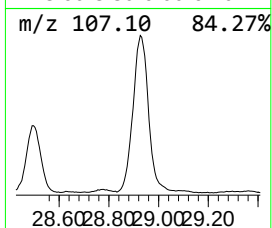
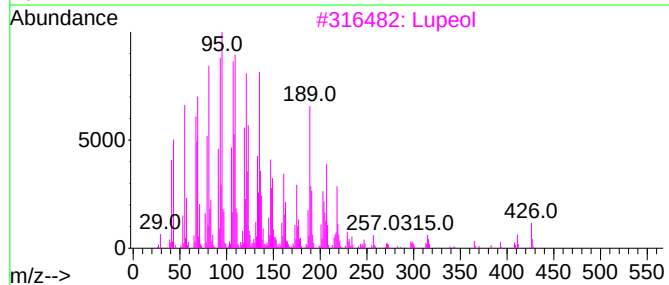
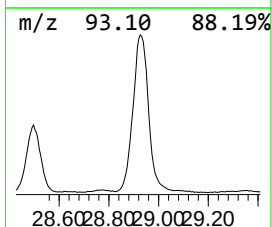
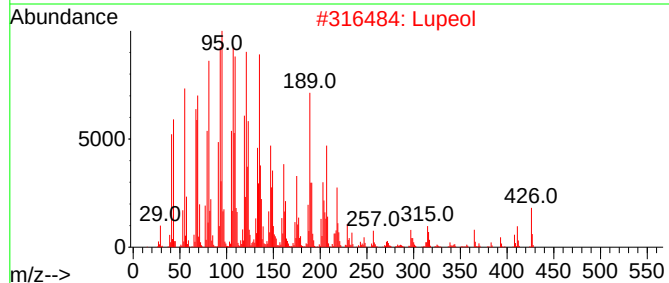
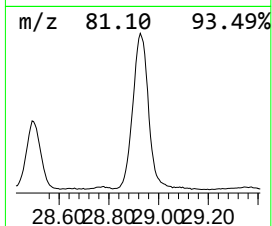
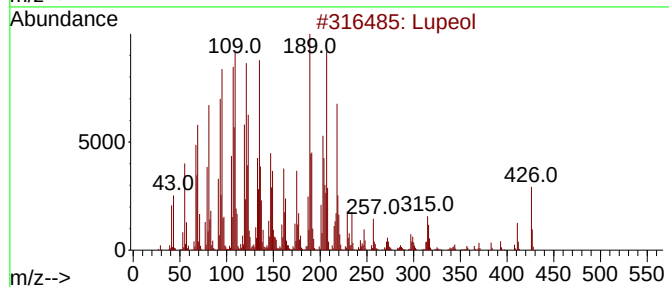
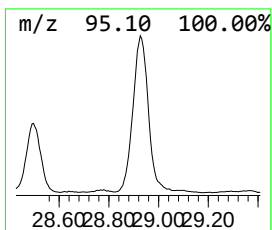
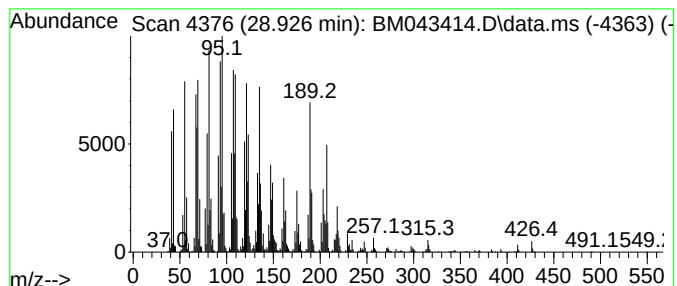
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Quant Title : SVOA CALIBRATION

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

Peak Number 21 Lupeol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.927	119.85 ng/ul	25682500	Perylene-d12	23.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	96
2			Lupeol	426	C30H50O	000545-47-1	95
3			Lupeol	426	C30H50O	000545-47-1	91
4			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	89
5			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043414.D
 Acq On : 19 Dec 2023 04:23
 Operator : MA/JU
 Sample : 05807-11
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AZ3

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
Butanoic acid	4.181	49.8	ng/ul	7473050	1	7.993	3002510	20.0
n-Hexadecanoic ...	18.268	7.4	ng/ul	1594940	4	17.363	4335620	20.0
Octadecanoic acid	19.539	2.9	ng/ul	621321	5	21.539	4346840	20.0
(DEL) Alkane: S...	21.256	17.9	ng/ul	3885730	5	21.539	4346840	20.0
unknown-01	21.451	4.9	ng/ul	1070160	5	21.539	4346840	20.0
(DEL) Alkane: C...	22.198	14.4	ng/ul	3139790	5	21.539	4346840	20.0
(DEL) Alkane: S...	23.256	15.0	ng/ul	3211420	6	23.962	4285670	20.0
1-Heneicosanol	23.303	5.6	ng/ul	1198170	6	23.962	4285670	20.0
(DEL) Alkane: S...	23.897	2.2	ng/ul	480345	6	23.962	4285670	20.0
.gamma.-Tocopherol	24.497	3.5	ng/ul	748139	6	23.962	4285670	20.0
2-Bromo dodecane	24.650	8.3	ng/ul	1786190	6	23.962	4285670	20.0
(DEL) Alkane: S...	24.744	7.5	ng/ul	1604590	6	23.962	4285670	20.0
Benzene, 1,4-bi...	24.874	10.2	ng/ul	2181220	6	23.962	4285670	20.0
unknown-02	26.350	6.4	ng/ul	1370490	6	23.962	4285670	20.0
4-n-Hexylthiane...	26.715	11.8	ng/ul	2528750	6	23.962	4285670	20.0
Valerena-4,7(11...	27.656	64.0	ng/ul	13707600	6	23.962	4285670	20.0
5-Bromo-4-oxo-4...	28.097	61.8	ng/ul	13241500	6	23.962	4285670	20.0
Lup-20(29)-en-3...	28.497	48.1	ng/ul	10314400	6	23.962	4285670	20.0
Lupeol	28.927	119.8	ng/ul	25682500	6	23.962	4285670	20.0