

Data Path : Z:\HPCHEM1\BNA G\DATA\BG081017\
 Data File : BG028271.D
 Acq On : 10 Aug 2017 23:19
 Operator : SJ/JU
 Sample : I4529-18
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AB9

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 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: 1

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.776	30	32	38	rBV4	1993	3456	0.30%	0.022%
2	3.853	40	45	56	rVB6	6711	15343	1.31%	0.099%
3	4.622	172	176	181	rVB5	2070	3744	0.32%	0.024%
4	4.769	198	201	207	rVB4	6365	7642	0.65%	0.050%
5	5.175	264	270	277	rBV5	2581	4581	0.39%	0.030%
6	5.474	319	321	327	rVB2	2442	3628	0.31%	0.024%
7	6.444	479	486	492	rBV6	2915	6448	0.55%	0.042%
8	6.884	555	561	566	rVB4	6132	9402	0.80%	0.061%
9	6.996	572	580	582	rVV4	2127	4492	0.38%	0.029%
10	7.043	582	588	593	rVB4	9022	16108	1.38%	0.104%
11	7.343	631	639	646	rVB5	14192	25458	2.18%	0.165%
12	7.501	657	666	680	rBV2	148618	324358	27.73%	2.102%
13	7.672	686	695	706	rBV	103039	187959	16.07%	1.218%
14	7.772	706	712	714	rVV4	2070	3047	0.26%	0.020%
15	7.883	722	731	747	rVB	142502	260353	22.26%	1.687%
16	8.353	804	811	823	rBV	179188	324424	27.73%	2.102%
17	8.482	830	833	838	rVB3	2287	3480	0.30%	0.023%
18	8.559	838	846	851	rVV2	2595	6296	0.54%	0.041%
19	8.612	851	855	865	rVB6	2917	5952	0.51%	0.039%
20	9.047	920	929	940	rBV	187541	345354	29.52%	2.238%
21	9.522	1002	1010	1019	rBV2	143658	271172	23.18%	1.757%
22	10.245	1124	1133	1143	rBV2	121293	234290	20.03%	1.518%
23	10.574	1181	1189	1198	rVB3	22520	41714	3.57%	0.270%
24	10.715	1207	1213	1217	rBV3	2027	4162	0.36%	0.027%
25	10.786	1217	1225	1239	rBV2	182822	362186	30.96%	2.347%
26	10.933	1245	1250	1254	rBV3	6024	8418	0.72%	0.055%
27	11.168	1283	1290	1303	rVB	264420	505083	43.18%	3.273%
28	11.303	1303	1313	1327	rBV3	145896	304145	26.00%	1.971%
29	12.331	1479	1488	1493	rBV3	4878	9413	0.80%	0.061%
30	12.495	1509	1516	1522	rBV2	8946	14107	1.21%	0.091%
31	12.619	1532	1537	1547	rVB3	3515	7162	0.61%	0.046%
32	12.748	1553	1559	1563	rVB4	2500	4686	0.40%	0.030%
33	13.312	1650	1655	1659	rBV3	2226	4517	0.39%	0.029%
34	13.559	1693	1697	1700	rVB3	2778	3220	0.28%	0.021%

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35	13.982	1767	1769	1775	rBV2	2179	3275	0.28%	0.021%
36	14.276	1814	1819	1823	rVB2	3053	4397	0.38%	0.028%
37	14.346	1823	1831	1836	rBV	389232	578823	49.48%	3.751%
38	14.393	1836	1839	1847	rVB	113633	151151	12.92%	0.979%
39	14.652	1874	1883	1893	rBV	376669	636102	54.38%	4.122%
40	14.810	1905	1910	1915	rVB4	2882	5031	0.43%	0.033%
41	14.957	1926	1935	1945	rBV2	461040	757279	64.74%	4.907%
42	15.151	1960	1968	1984	rBV2	74682	189863	16.23%	1.230%
43	15.345	1998	2001	2002	rBV3	3658	3073	0.26%	0.020%
44	15.721	2060	2065	2068	rBV4	3353	6323	0.54%	0.041%
45	15.756	2068	2071	2077	rVB3	9625	13524	1.16%	0.088%
46	15.944	2092	2103	2112	rBV	554128	856452	73.22%	5.550%
47	16.056	2112	2122	2134	rBV2	151156	244697	20.92%	1.586%
48	16.179	2138	2143	2150	rVB7	7859	16289	1.39%	0.106%
49	16.314	2163	2166	2169	rVB3	3020	3545	0.30%	0.023%
50	16.379	2169	2177	2183	rBV5	3824	9580	0.82%	0.062%
51	16.455	2183	2190	2195	rVV4	4534	8255	0.71%	0.053%
52	16.626	2214	2219	2232	rVV5	25877	58635	5.01%	0.380%
53	16.908	2260	2267	2270	rVB4	2300	3695	0.32%	0.024%
54	16.973	2273	2278	2281	rBV5	4214	6237	0.53%	0.040%
55	17.072	2291	2295	2299	rBV5	4408	8014	0.69%	0.052%
56	17.419	2350	2354	2358	rVB2	8570	8691	0.74%	0.056%
57	17.707	2395	2403	2412	rBV	604578	969928	82.92%	6.285%
58	17.807	2412	2420	2429	rVB	613538	958609	81.95%	6.212%
59	17.960	2440	2446	2451	rVB7	4544	8583	0.73%	0.056%
60	18.024	2451	2457	2462	rBV5	3260	8128	0.69%	0.053%
61	18.159	2476	2480	2482	rVB3	3613	4545	0.39%	0.029%
62	18.336	2503	2510	2518	rBV7	4099	8026	0.69%	0.052%
63	18.406	2518	2522	2524	rVB3	2508	3145	0.27%	0.020%
64	18.447	2524	2529	2531	rBV4	4229	6197	0.53%	0.040%
65	18.559	2541	2548	2559	rBV	76127	155460	13.29%	1.007%
66	18.718	2573	2575	2579	rBV5	2694	4058	0.35%	0.026%
67	18.835	2591	2595	2599	rVB4	3342	4350	0.37%	0.028%
68	18.876	2599	2602	2607	rVB5	3515	5348	0.46%	0.035%
69	19.041	2628	2630	2636	rBV4	2785	5853	0.50%	0.038%
70	19.211	2651	2659	2661	rBV7	4366	8433	0.72%	0.055%
71	19.493	2698	2707	2716	rBV7	35096	58855	5.03%	0.381%

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72	19.711	2734	2744	2750	rBV3	13110	34155	2.92%	0.221%
73	19.816	2756	2762	2776	rBV2	116672	213435	18.25%	1.383%
74	19.969	2784	2788	2795	rVB7	11419	23899	2.04%	0.155%
75	20.081	2799	2807	2821	rVB	768429	1136700	97.18%	7.366%
76	20.557	2886	2888	2893	rBV4	6979	8485	0.73%	0.055%
77	20.903	2946	2947	2949	rBV	3797	3589	0.31%	0.023%
78	20.938	2951	2953	2955	rBV3	5657	4643	0.40%	0.030%
79	20.997	2961	2963	2969	rVB6	7597	9053	0.77%	0.059%
80	21.068	2970	2975	2981	rBV5	9931	17641	1.51%	0.114%
81	21.379	3018	3028	3041	rVB8	19785	73906	6.32%	0.479%
82	21.608	3062	3067	3073	rBV6	15537	26571	2.27%	0.172%
83	21.873	3108	3112	3117	rVB7	6840	7482	0.64%	0.048%
84	22.037	3132	3140	3152	rBV	641641	1123749	96.07%	7.282%
85	22.313	3186	3187	3190	rBV3	3965	4408	0.38%	0.029%
86	22.848	3272	3278	3281	rBV5	13553	20308	1.74%	0.132%
87	23.541	3393	3396	3397	rBV3	3936	3486	0.30%	0.023%
88	23.594	3400	3405	3412	rVB7	14427	23565	2.01%	0.153%
89	23.806	3435	3441	3448	rVB8	12456	29587	2.53%	0.192%
90	24.464	3544	3553	3562	rBV2	113509	263121	22.49%	1.705%
91	25.298	3682	3695	3711	rVB2	360152	1094379	93.56%	7.092%
92	25.533	3719	3735	3752	rVB3	327136	1169732	100.00%	7.580%
93	26.597	3913	3916	3917	rBV3	5751	6004	0.51%	0.039%
94	26.714	3926	3936	3949	rVB2	138021	437269	37.38%	2.834%
95	26.867	3952	3962	3973	rBV5	47185	154937	13.25%	1.004%
96	28.195	4178	4188	4199	rVB4	38380	136031	11.63%	0.881%
97	29.129	4345	4347	4350	rBV4	4018	5305	0.45%	0.034%
98	29.329	4380	4381	4384	rBV3	6272	4941	0.42%	0.032%
99	29.981	4480	4492	4506	rVB5	41237	177322	15.16%	1.149%
100	32.125	4847	4857	4870	rVB9	22320	100119	8.56%	0.649%

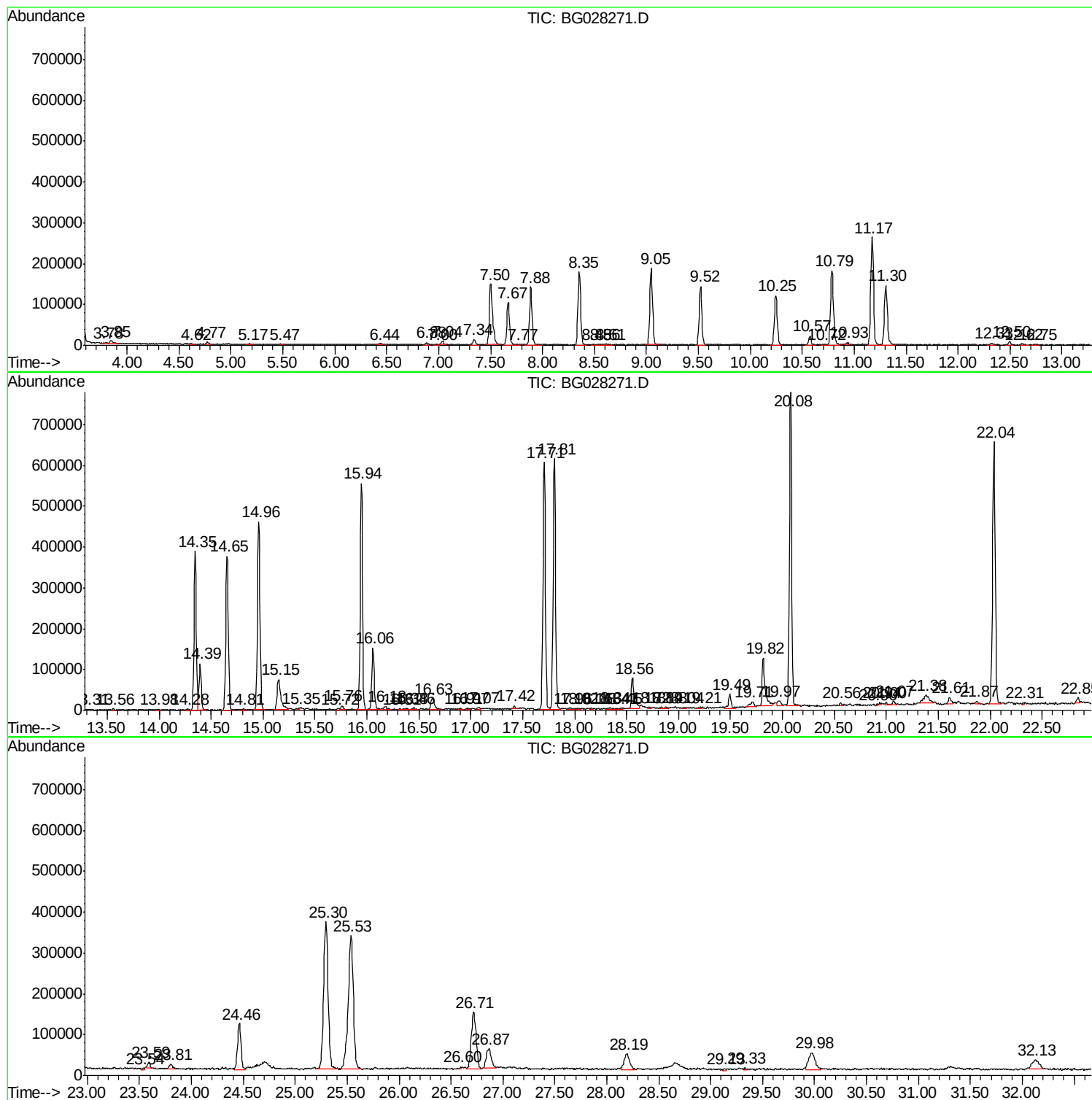
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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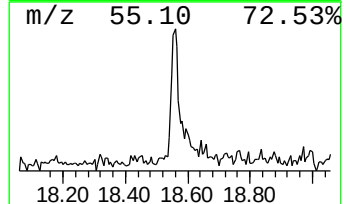
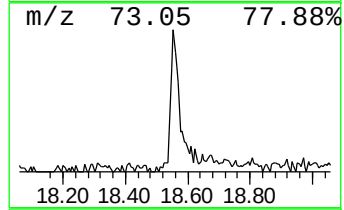
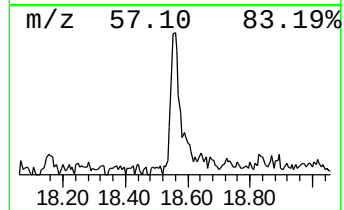
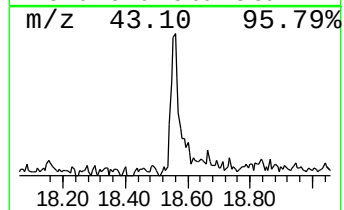
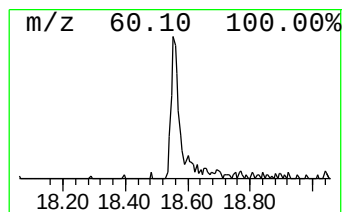
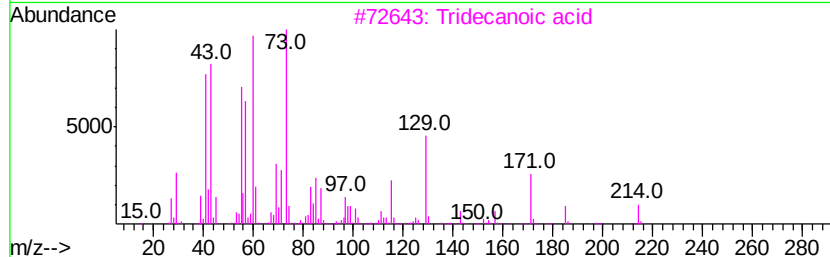
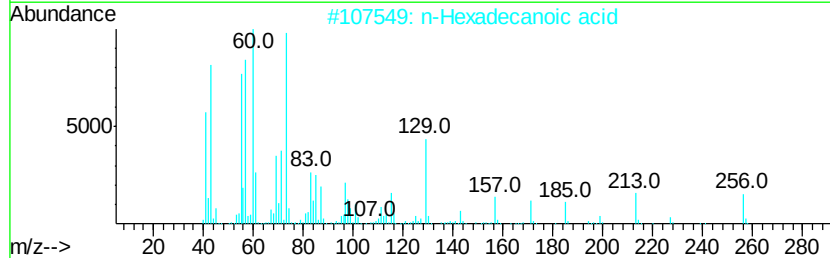
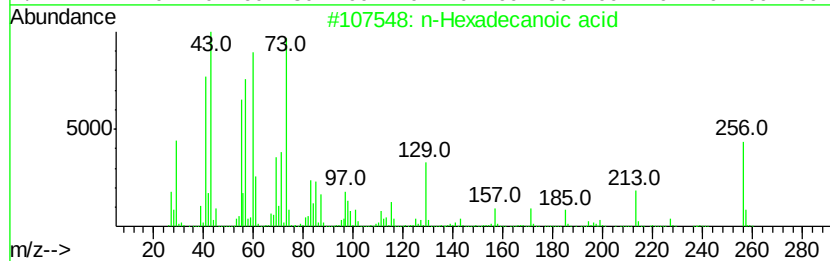
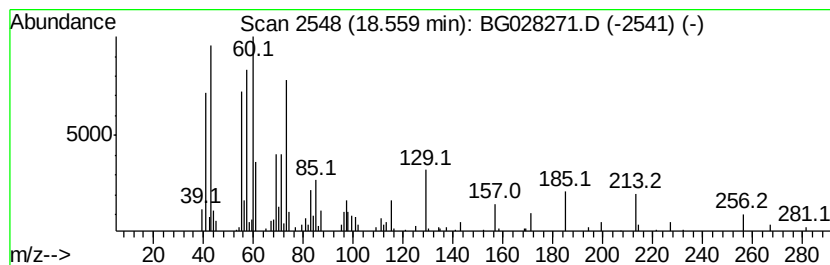
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.56	3.21 ng/ul	155460	Phenanthrene-d10	17.71		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	46
5		Nonanoic acid	158	C9H18O2	000112-05-0	38



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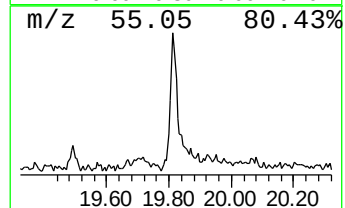
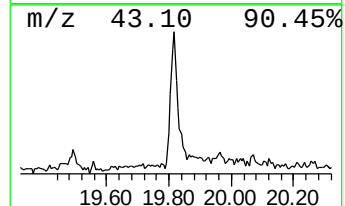
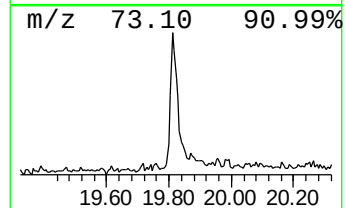
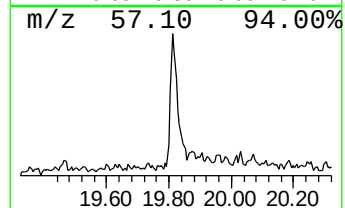
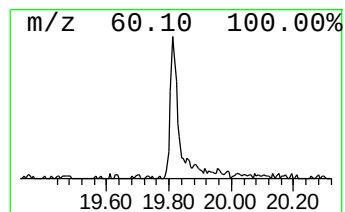
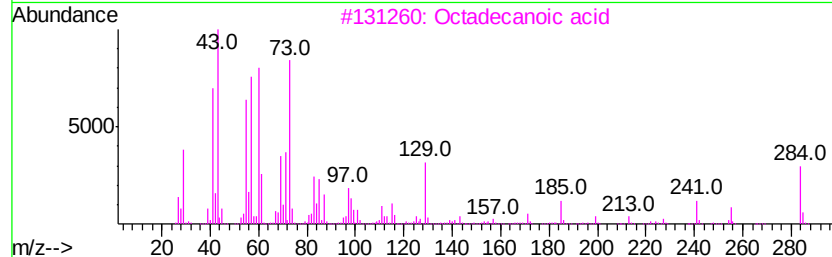
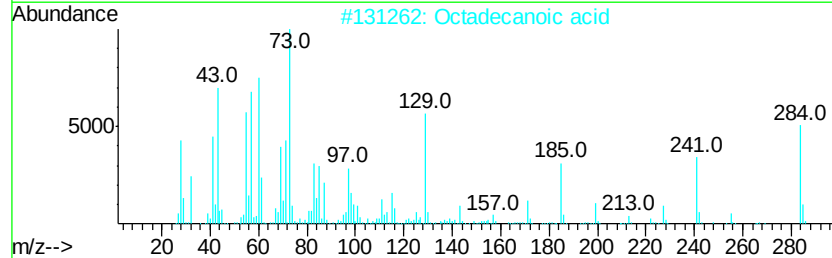
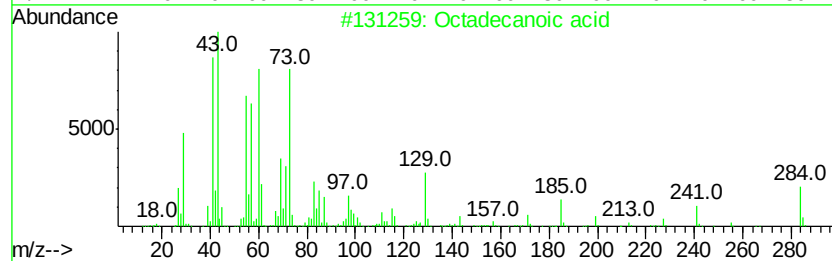
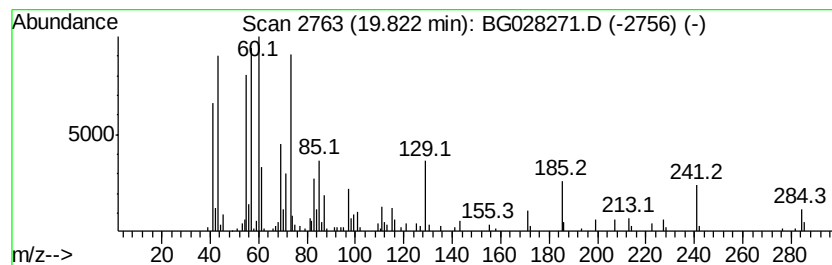
Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	4.40 ng/ul	213435	Phenanthrene-d10	17.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Octadecanoic acid	284	C18H36O2	000057-11-4	96
3		Octadecanoic acid	284	C18H36O2	000057-11-4	95
4		Octadecanoic acid	284	C18H36O2	000057-11-4	94
5		Octadecanoic acid	284	C18H36O2	000057-11-4	93



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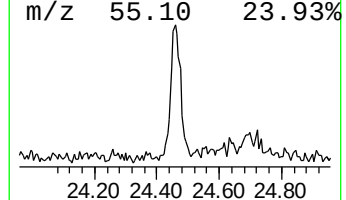
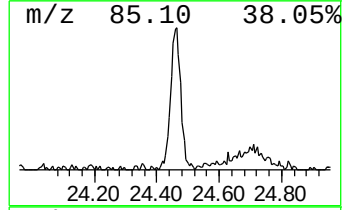
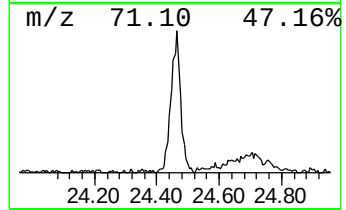
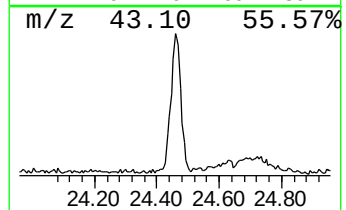
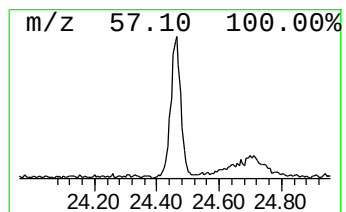
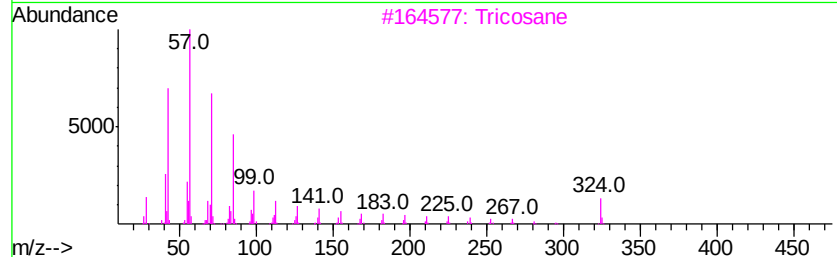
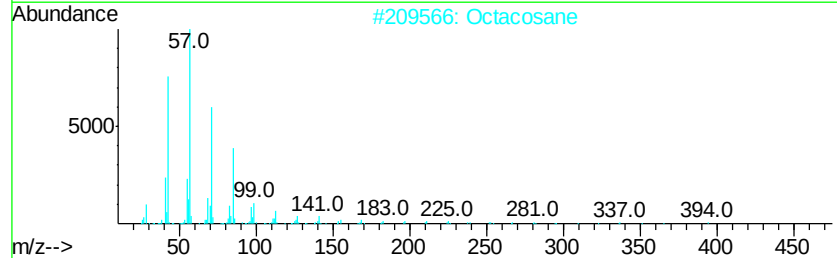
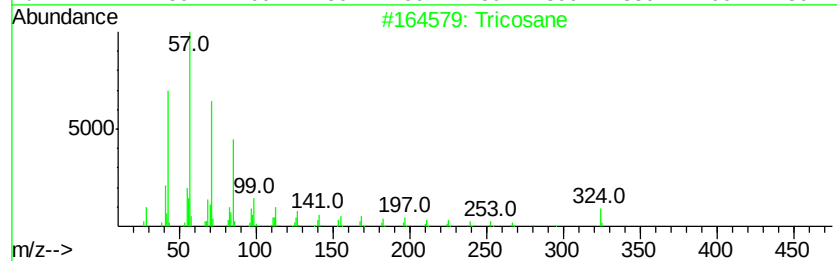
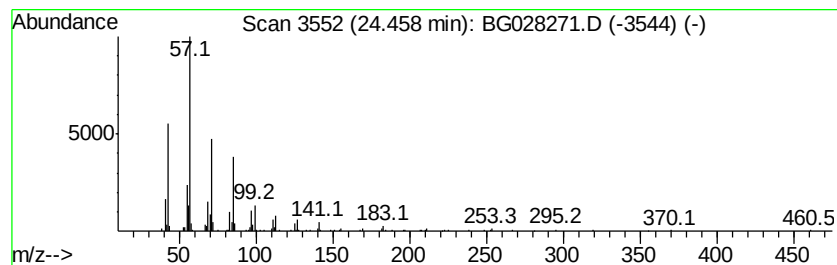
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TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.46	4.50 ng/ul	263121	Perylene-d12	25.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	93
2			Octacosane	394	C28H58	000630-02-4	90
3			Tricosane	324	C23H48	000638-67-5	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Heptacosane	380	C27H56	000593-49-7	87



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ClientSampleId :
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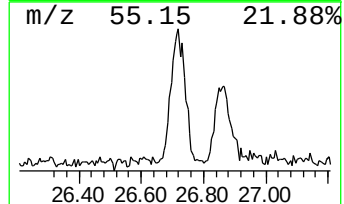
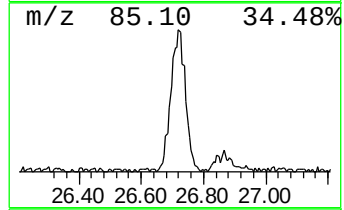
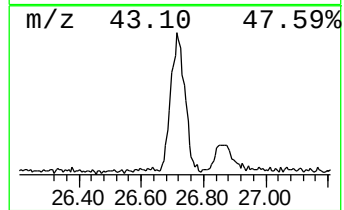
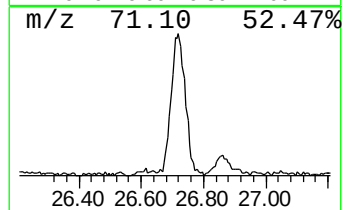
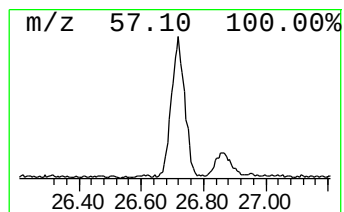
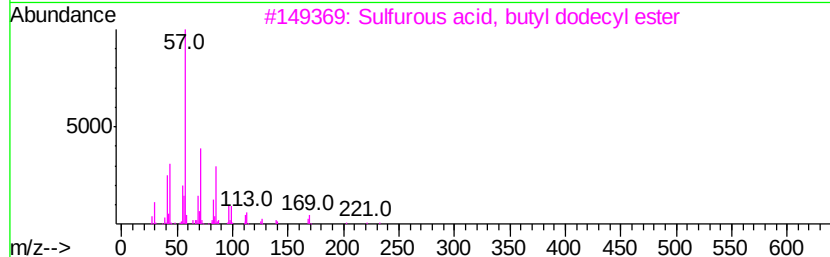
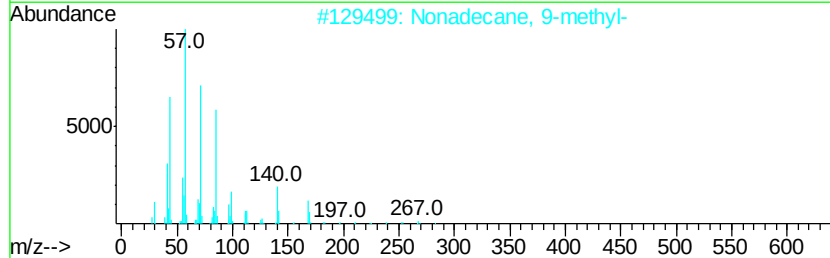
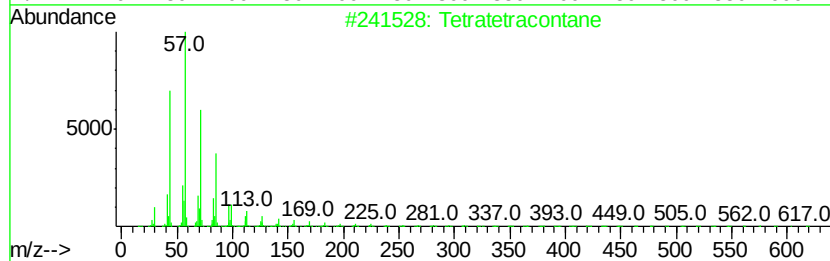
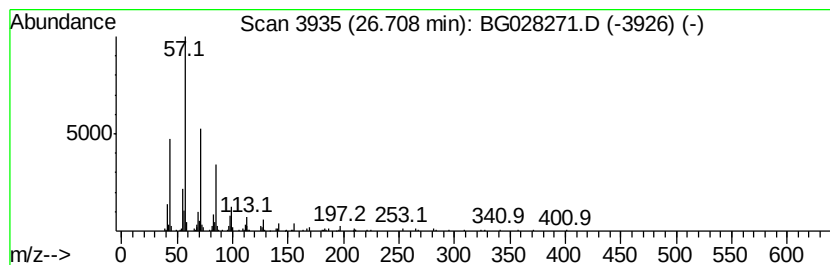
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.71	7.48 ng/ul	437269	Perylene-d12	25.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	87
4		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA G\DATA\BG081017\
Data File : BG028271.D
Acq On : 10 Aug 2017 23:19
Operator : SJ/JU
Sample : I4529-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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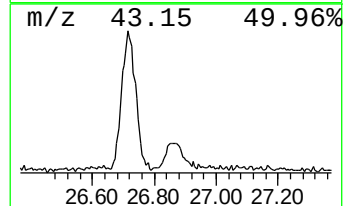
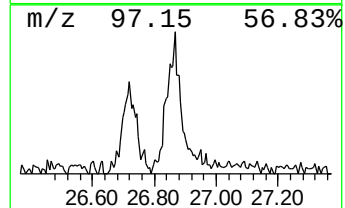
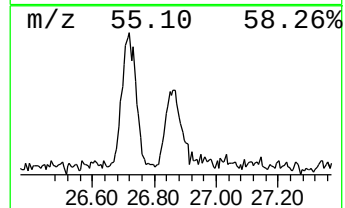
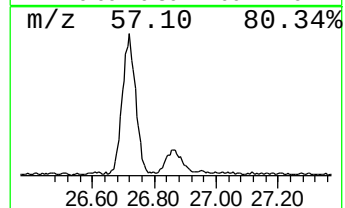
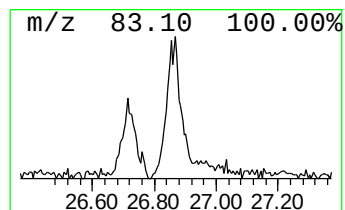
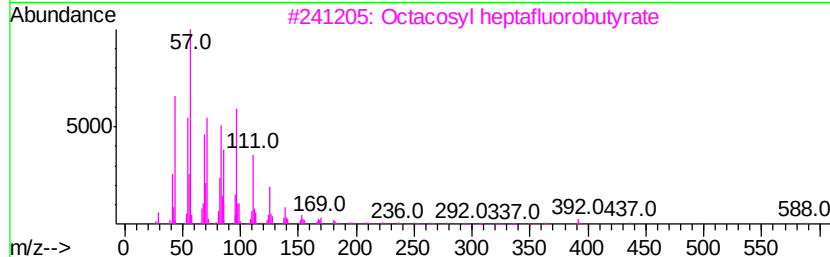
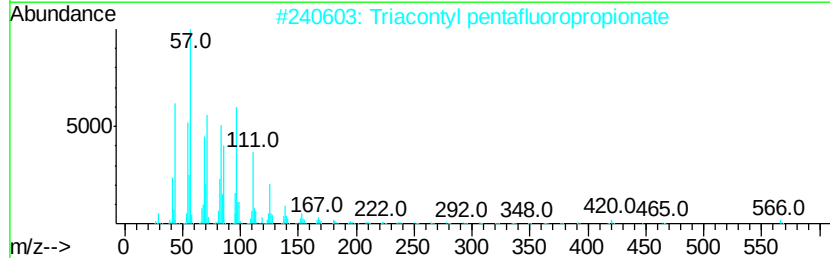
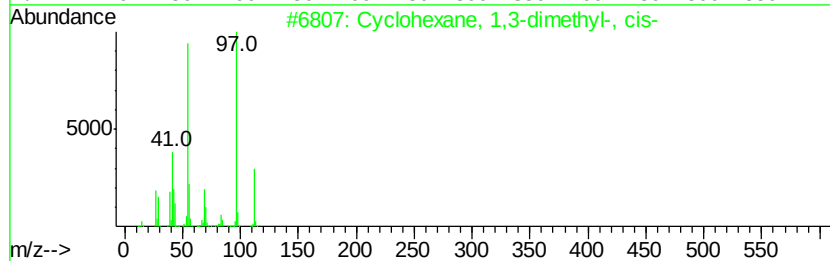
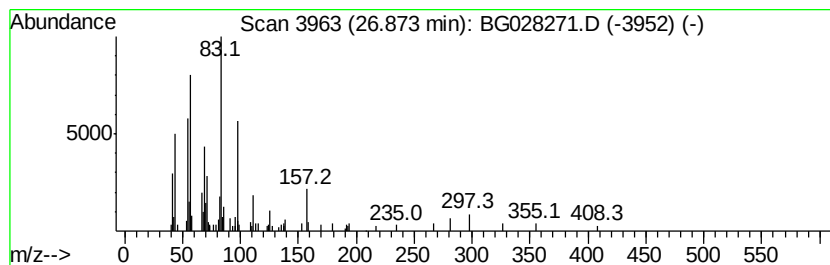
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Cyclic26.87 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.87	2.65 ng/ul	154937	Perylene-d12	25.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	22
2		Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	20
3		Octacosyl heptafluorobutylate	606	C32H57F7O2	1000351-83-6	20
4		Triacetyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	20
5		Dotriacetyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	20



Data Path : Z:\HPCHEM1\BNA G\DATA\BG081017\
Data File : BG028271.D
Acq On : 10 Aug 2017 23:19
Operator : SJ/JU
Sample : I4529-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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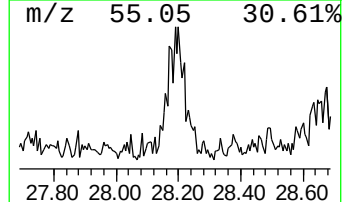
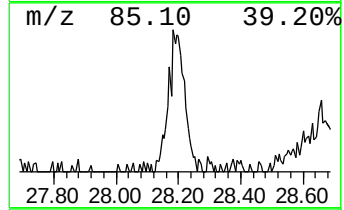
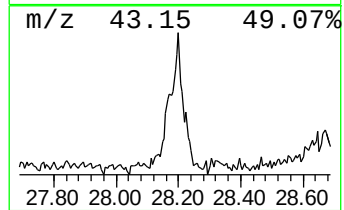
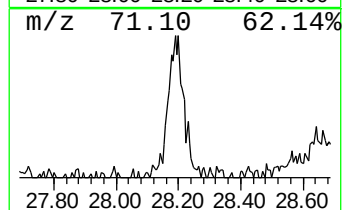
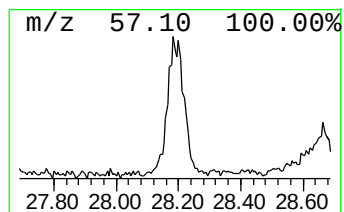
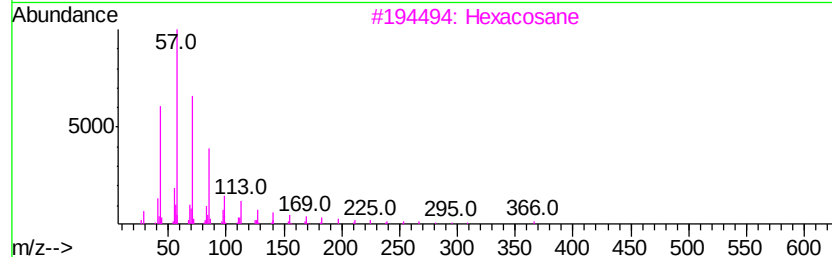
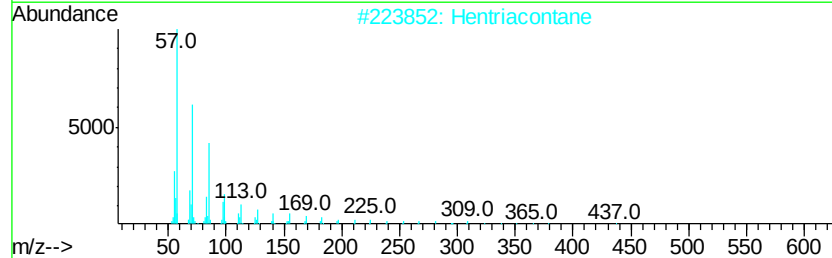
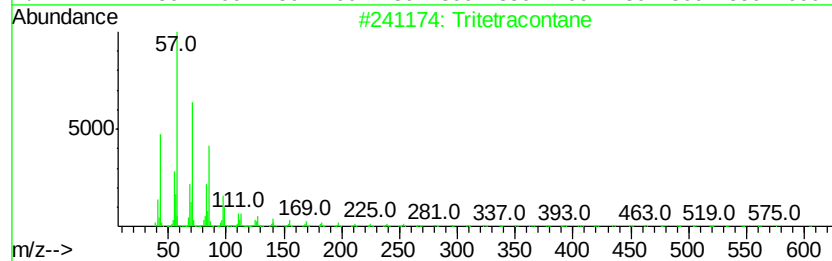
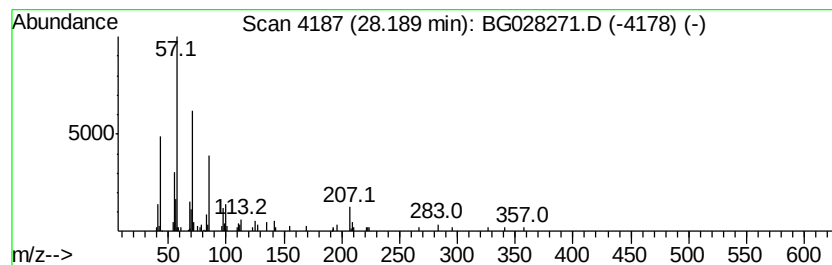
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
28.19	2.33 ng/ul	136031	Perylene-d12	25.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tritetracontane	605	C43H88	007098-21-7	68
2		Hentriacontane	437	C31H64	000630-04-6	64
3		Hexacosane	366	C26H54	000630-01-3	58
4		Tetradecane	198	C14H30	000629-59-4	52
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	52



Data Path : Z:\HPCHEM1\BNA G\DATA\BG081017\
Data File : BG028271.D
Acq On : 10 Aug 2017 23:19
Operator : SJ/JU
Sample : I4529-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

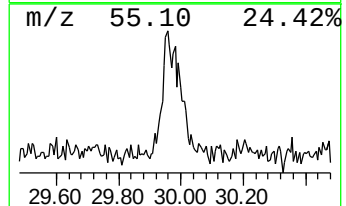
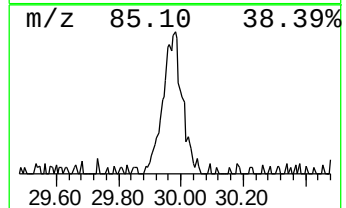
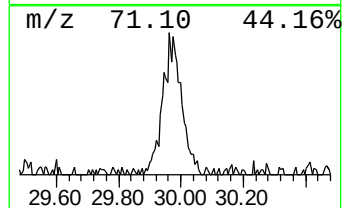
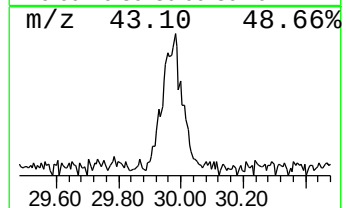
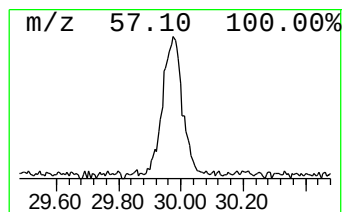
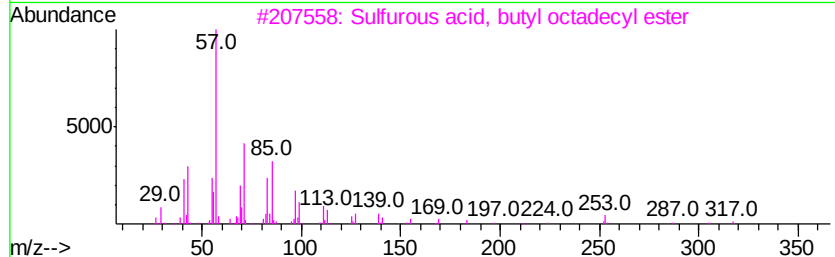
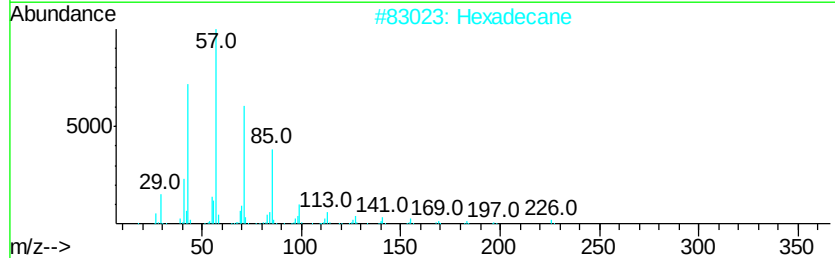
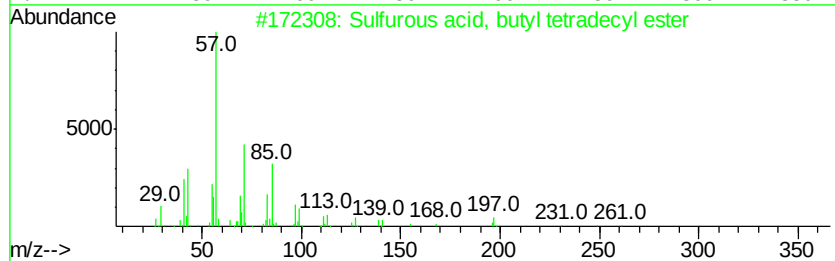
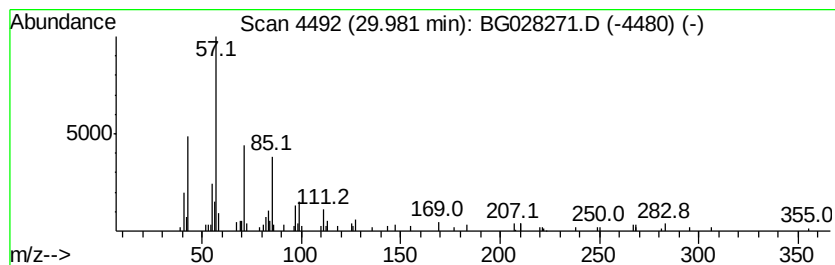
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Sulfurous acid, butyl tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
29.98	3.03 ng/ul	177322	Perylene-d12	25.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
2	Hexadecane	226	C16H34	000544-76-3	64
3	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	64
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64
5	Di-n-decylsulfone	346	C20H42O2S	111530-37-1	59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081017\
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Acq On : 10 Aug 2017 23:19
Operator : SJ/JU
Sample : I4529-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic acid	18.56	3.2	ng/ul	155460	4	17.71	969928	20.0
Octadecanoic acid	19.82	4.4	ng/ul	213435	4	17.71	969928	20.0
(DEL) Alkane: Str...	24.46	4.5	ng/ul	263121	6	25.54	1169730	20.0
(DEL) Alkane: Str...	26.71	7.5	ng/ul	437269	6	25.54	1169730	20.0
(DEL) Alkane: Cyc...	26.87	2.6	ng/ul	154937	6	25.54	1169730	20.0
(DEL) Alkane: Str...	28.19	2.3	ng/ul	136031	6	25.54	1169730	20.0
Sulfurous acid, b...	29.98	3.0	ng/ul	177322	6	25.54	1169730	20.0