

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
 Data File : BG027506.D
 Acq On : 17 Jun 2017 13:52
 Operator : SJ/MA
 Sample : I3599-20
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 F5D38

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-BG061617.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	4.076	27	32	43	rVB3	8173	16057	1.19%	0.099%
2	4.352	72	79	90	rVB6	2223	7440	0.55%	0.046%
3	6.614	458	464	468	rBV4	1827	3568	0.27%	0.022%
4	6.738	480	485	492	rBV3	1677	3085	0.23%	0.019%
5	7.460	595	608	616	rVB7	3686	9039	0.67%	0.056%
6	7.654	632	641	656	rBV	153605	297515	22.13%	1.839%
7	7.830	661	671	684	rBV	127750	222534	16.56%	1.375%
8	8.054	700	709	717	rVB	143582	266363	19.82%	1.646%
9	8.518	780	788	800	rVB	161085	291452	21.68%	1.801%
10	8.841	840	843	852	rVB5	1542	3030	0.23%	0.019%
11	9.194	894	903	914	rBV	196712	353235	26.28%	2.183%
12	9.681	977	986	993	rVV	147614	278703	20.73%	1.723%
13	9.734	993	995	1003	rVB2	5572	9396	0.70%	0.058%
14	10.404	1098	1109	1119	rBV2	121034	232379	17.29%	1.436%
15	10.580	1133	1139	1150	rBV4	2978	5955	0.44%	0.037%
16	10.944	1192	1201	1210	rBV	183491	353476	26.30%	2.185%
17	11.338	1260	1268	1279	rVB	253370	485309	36.11%	3.000%
18	11.461	1279	1289	1307	rBV	184416	367888	27.37%	2.274%
19	11.785	1337	1344	1349	rBV3	1478	3517	0.26%	0.022%
20	12.760	1505	1510	1522	rBV4	1916	3669	0.27%	0.023%
21	12.883	1527	1531	1538	rVB3	2873	5263	0.39%	0.033%
22	13.348	1603	1610	1614	rBV4	2335	3740	0.28%	0.023%
23	13.453	1624	1628	1639	rVB5	2914	5391	0.40%	0.033%
24	13.694	1664	1669	1675	rBV3	4494	6989	0.52%	0.043%
25	14.487	1795	1804	1809	rBV	415184	640988	47.69%	3.962%
26	14.534	1809	1812	1819	rVV	194561	272897	20.30%	1.687%
27	14.799	1848	1857	1872	rBV	423910	718381	53.45%	4.440%
28	14.957	1877	1884	1890	rBV3	6811	10056	0.75%	0.062%
29	15.104	1898	1909	1918	rBV2	427411	732916	54.53%	4.530%
30	15.269	1924	1937	1954	rBV	186546	342828	25.51%	2.119%
31	15.392	1954	1958	1965	rVV6	1990	4271	0.32%	0.026%
32	15.469	1965	1971	1983	rVV3	16163	37404	2.78%	0.231%
33	15.574	1983	1989	1996	rVB7	2810	6595	0.49%	0.041%
34	15.639	1996	2000	2006	rBV6	1659	3059	0.23%	0.019%

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35	15.862	2033	2038	2041	rBV4	2780	4804	0.36%	0.030%
36	15.903	2041	2045	2050	rVB2	17141	22866	1.70%	0.141%
37	15.968	2050	2056	2059	rVB4	1971	3669	0.27%	0.023%
38	16.009	2059	2063	2069	rBV5	2216	3507	0.26%	0.022%
39	16.091	2069	2077	2087	rBV	610012	973523	72.43%	6.017%
40	16.191	2087	2094	2103	rVV	216502	338915	25.21%	2.095%
41	16.326	2103	2117	2125	rVV8	7803	22816	1.70%	0.141%
42	16.409	2125	2131	2134	rBV5	2538	4425	0.33%	0.027%
43	16.456	2134	2139	2145	rVV5	2426	4369	0.33%	0.027%
44	16.526	2145	2151	2156	rVB5	3222	4363	0.32%	0.027%
45	16.761	2187	2191	2199	rBV	19972	33620	2.50%	0.208%
46	17.102	2247	2249	2253	rBV4	1989	2925	0.22%	0.018%
47	17.202	2264	2266	2274	rVV6	3096	6179	0.46%	0.038%
48	17.272	2274	2278	2283	rVB4	3328	4367	0.32%	0.027%
49	17.343	2284	2290	2293	rVB5	2137	3348	0.25%	0.021%
50	17.402	2293	2300	2303	rBV8	2350	4959	0.37%	0.031%
51	17.560	2320	2327	2333	rBV2	14267	21093	1.57%	0.130%
52	17.619	2333	2337	2339	rBV5	2603	3570	0.27%	0.022%
53	17.854	2370	2377	2387	rBV2	590959	952838	70.89%	5.889%
54	17.954	2387	2394	2405	rVB	668963	1117695	83.15%	6.908%
55	18.095	2415	2418	2426	rVB6	2129	3902	0.29%	0.024%
56	18.301	2448	2453	2457	rBV	5580	8143	0.61%	0.050%
57	18.588	2495	2502	2506	rVB7	1807	4227	0.31%	0.026%
58	18.694	2510	2520	2532	rBV2	87854	169262	12.59%	1.046%
59	19.229	2605	2611	2614	rVB6	2155	4546	0.34%	0.028%
60	19.264	2614	2617	2622	rBV5	2310	3906	0.29%	0.024%
61	19.429	2640	2645	2648	rVV6	1751	3610	0.27%	0.022%
62	19.699	2688	2691	2697	rBV7	2003	4673	0.35%	0.029%
63	19.858	2707	2718	2729	rBV3	10348	33453	2.49%	0.207%
64	19.952	2730	2734	2742	rBV2	32251	61891	4.60%	0.383%
65	20.104	2756	2760	2767	rVB4	8500	16936	1.26%	0.105%
66	20.222	2767	2780	2791	rBV	843438	1344126	100.00%	8.308%
67	20.492	2820	2826	2829	rBV	52503	61609	4.58%	0.381%
68	20.527	2829	2832	2838	rVB	102958	114802	8.54%	0.710%
69	20.604	2842	2845	2848	rBV5	3718	4532	0.34%	0.028%
70	20.651	2848	2853	2856	rVV5	11320	14632	1.09%	0.090%
71	20.798	2875	2878	2882	rBV6	2431	3282	0.24%	0.020%

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72	20.850	2882	2887	2888	rBV5	2100	3594	0.27%	0.022%
73	21.056	2920	2922	2925	rVB4	3623	3952	0.29%	0.024%
74	21.156	2935	2939	2941	rBV4	8018	10682	0.79%	0.066%
75	21.197	2942	2946	2949	rVB2	8650	12607	0.94%	0.078%
76	21.538	2998	3004	3007	rBV3	33213	50678	3.77%	0.313%
77	21.579	3007	3011	3016	rVB	66051	87076	6.48%	0.538%
78	21.685	3026	3029	3035	rBV6	8300	13974	1.04%	0.086%
79	21.785	3040	3046	3073	rVB3	43632	144959	10.78%	0.896%
80	22.061	3089	3093	3097	rVB3	10936	12824	0.95%	0.079%
81	22.231	3113	3122	3129	rBV	566546	1096851	81.60%	6.779%
82	22.672	3193	3197	3204	rVB9	13413	23200	1.73%	0.143%
83	22.754	3205	3211	3216	rVV6	17298	32847	2.44%	0.203%
84	22.807	3216	3220	3229	rVB3	30629	50831	3.78%	0.314%
85	23.071	3260	3265	3275	rVB3	10408	22841	1.70%	0.141%
86	23.847	3390	3397	3406	rBV3	27749	62131	4.62%	0.384%
87	24.082	3431	3437	3444	rVB9	7955	17396	1.29%	0.108%
88	24.335	3477	3480	3487	rBV8	8801	18679	1.39%	0.115%
89	24.405	3487	3492	3501	rVB6	20111	47768	3.55%	0.295%
90	24.775	3547	3555	3564	rVB4	31524	74428	5.54%	0.460%
91	25.234	3632	3633	3637	rBV4	3094	4070	0.30%	0.025%
92	25.627	3687	3700	3714	rBV2	394181	1303351	96.97%	8.056%
93	25.786	3721	3727	3728	rBV6	10578	14842	1.10%	0.092%
94	25.886	3730	3744	3757	rVB2	327388	1199604	89.25%	7.414%
95	27.149	3949	3959	3972	rVB4	45364	153013	11.38%	0.946%
96	27.296	3981	3984	3987	rBV5	3192	4674	0.35%	0.029%
97	28.712	4212	4225	4241	rVB5	41148	164699	12.25%	1.018%
98	29.940	4432	4434	4436	rBV2	5474	4916	0.37%	0.030%
99	30.592	4533	4545	4560	rVB5	31691	141160	10.50%	0.872%
100	32.507	4869	4871	4876	rVB6	3915	6218	0.46%	0.038%

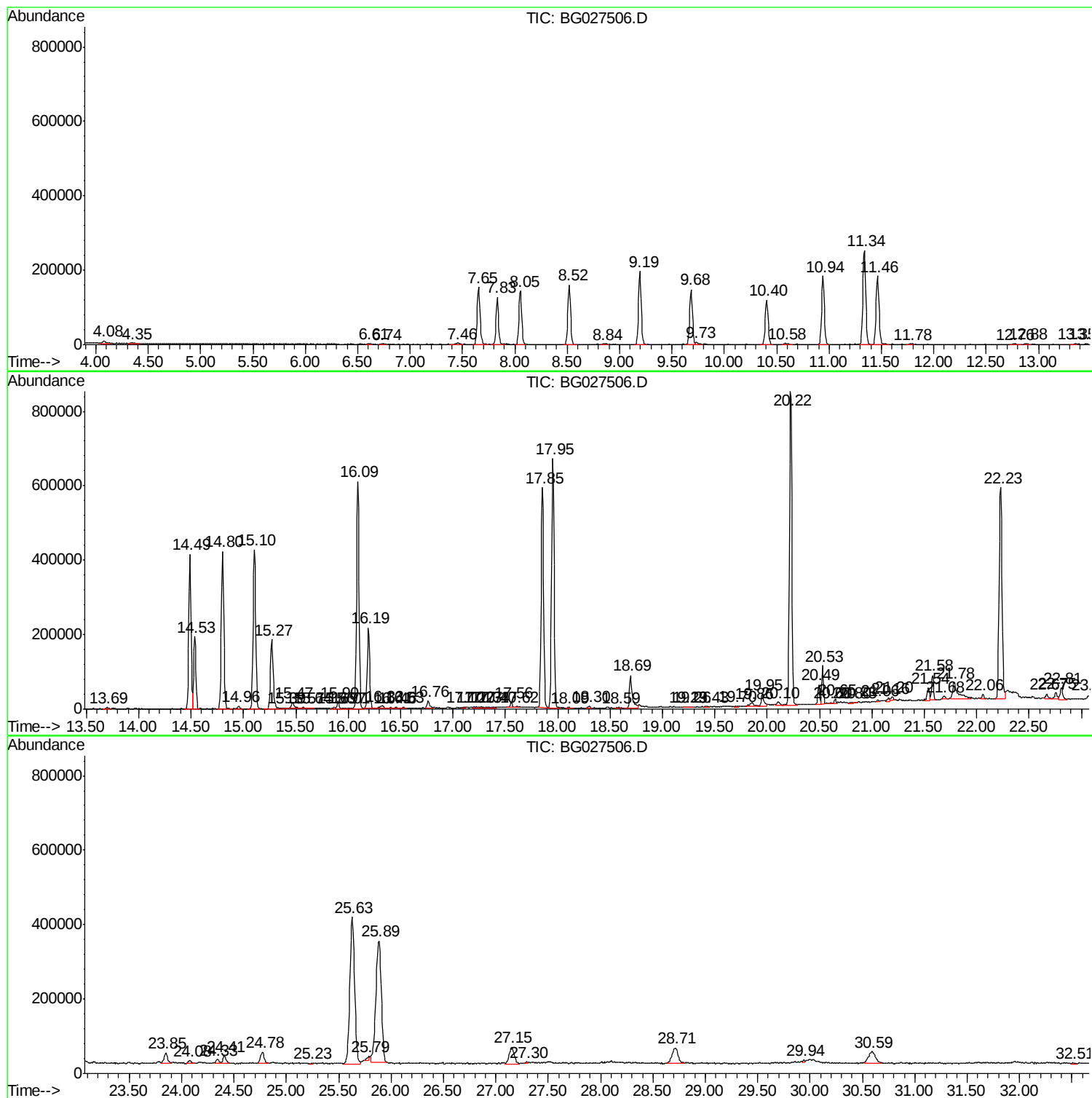
Sum of corrected areas: 16179636

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
Quant Title : SVOA CALIBRATION

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



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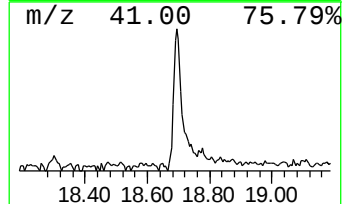
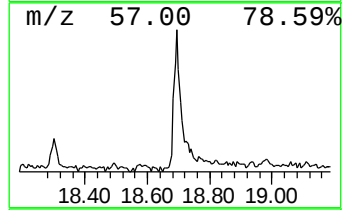
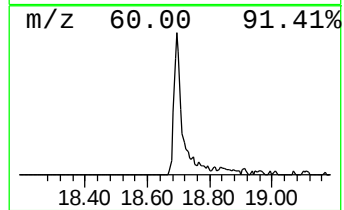
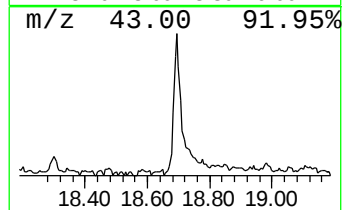
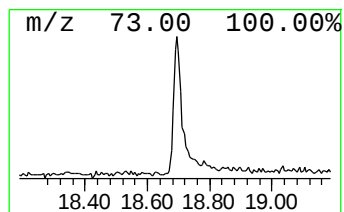
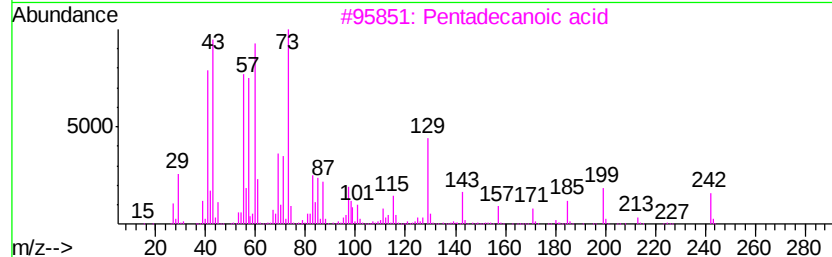
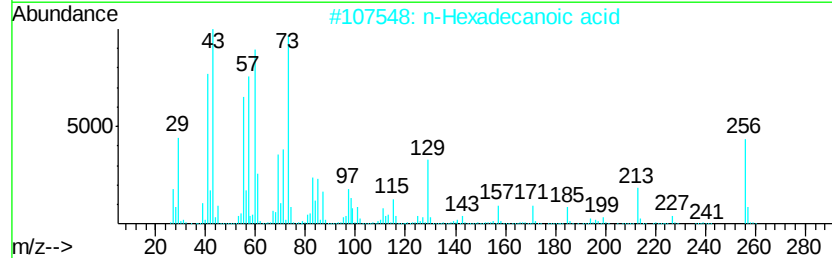
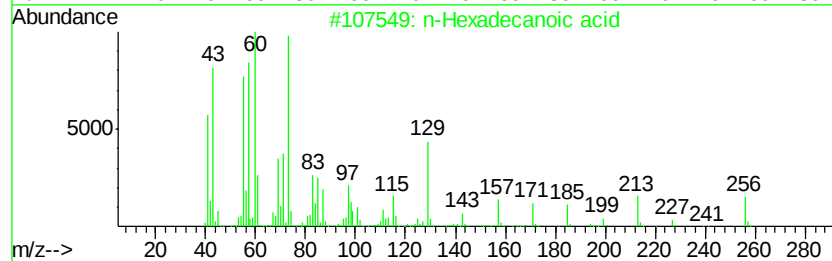
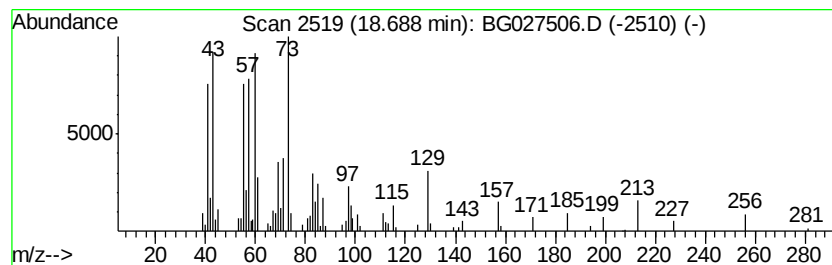
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.69	3.55 ng/ul	169262	Phenanthrene-d10	17.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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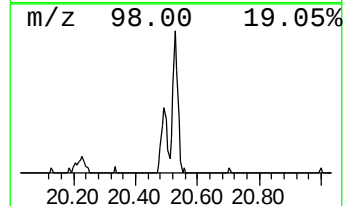
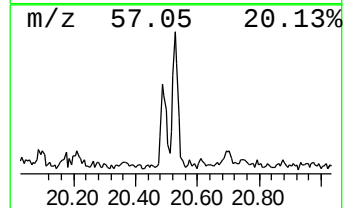
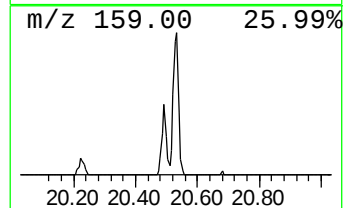
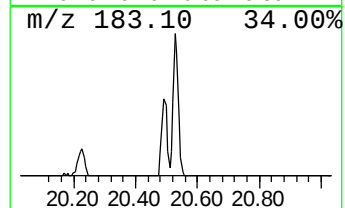
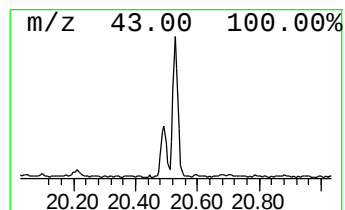
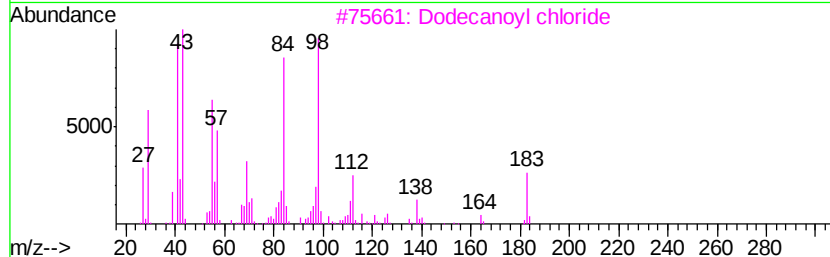
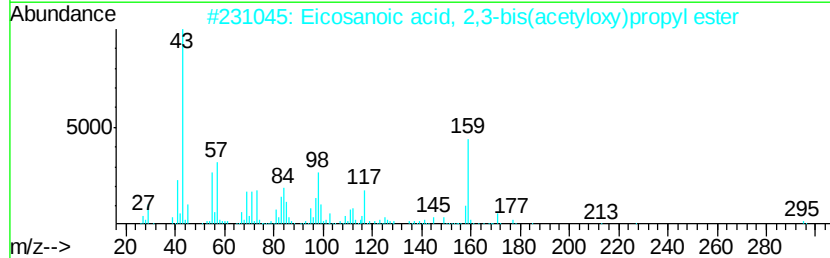
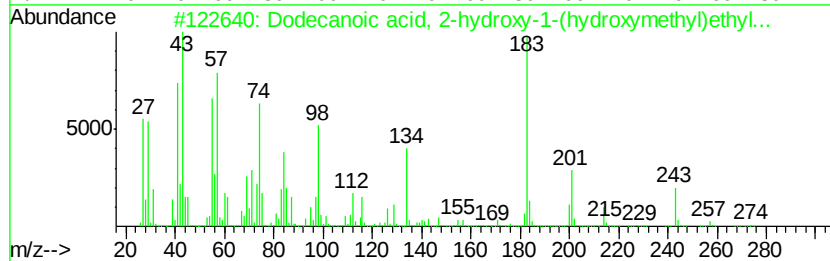
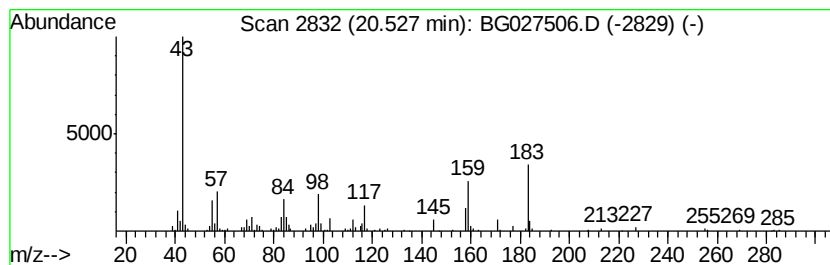
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.53	2.09 ng/ul	114802	Chrysene-d12	22.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	32
2		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	16
3		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	16
4		9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	12
5		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9



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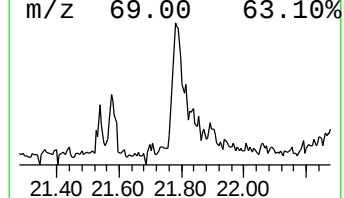
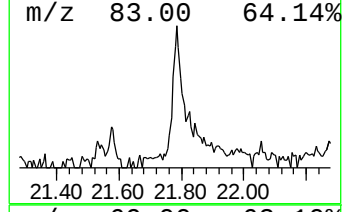
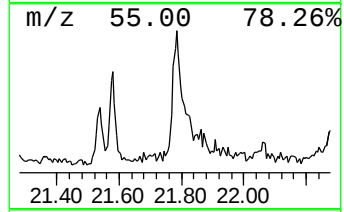
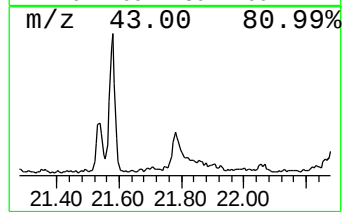
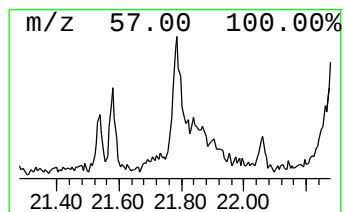
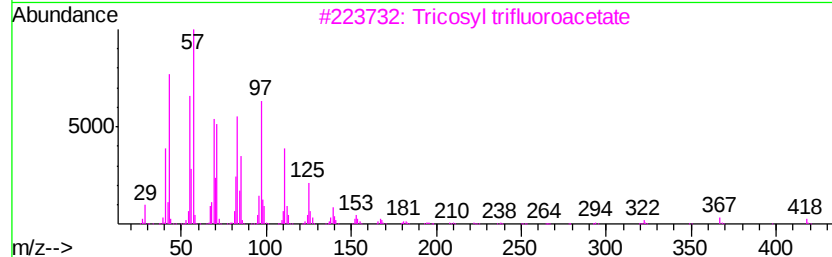
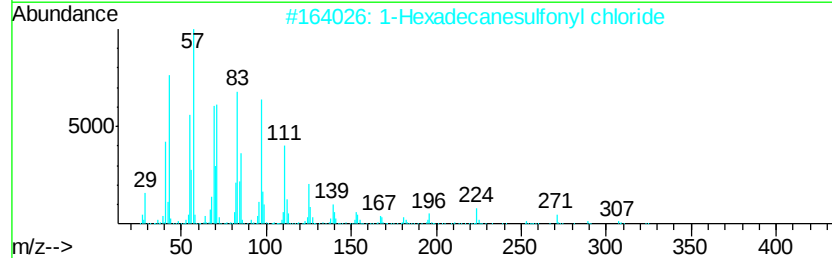
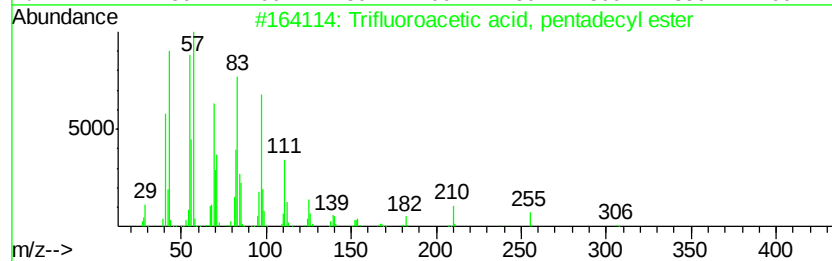
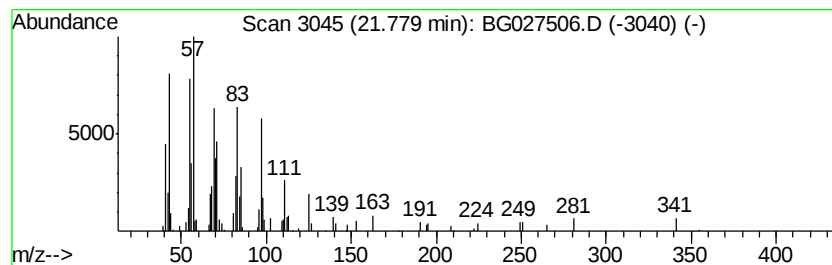
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Peak Number 3 Trifluoroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.78	2.64 ng/ul	144959	Chrysene-d12	22.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
2		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027506.D
Acq On : 17 Jun 2017 13:52
Operator : SJ/MA
Sample : I3599-20
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5D38

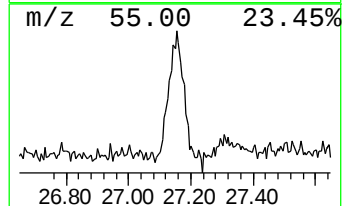
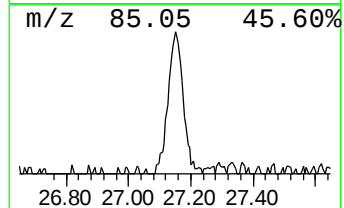
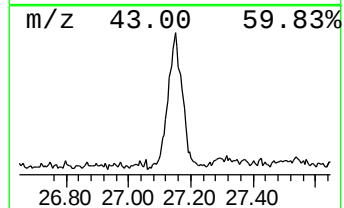
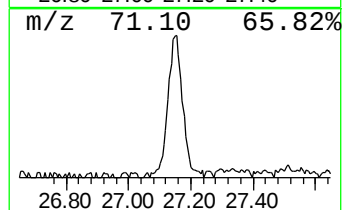
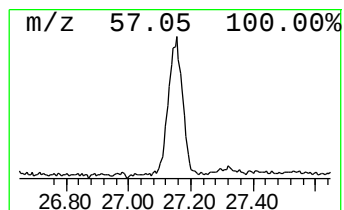
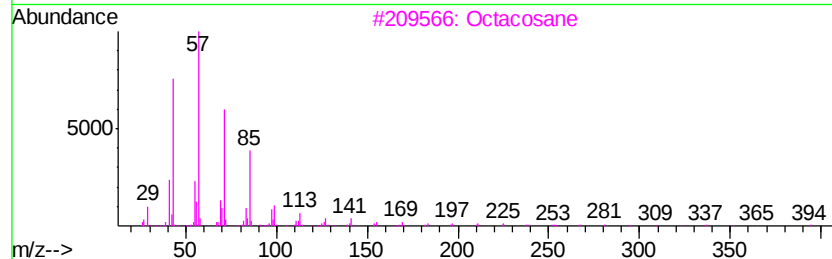
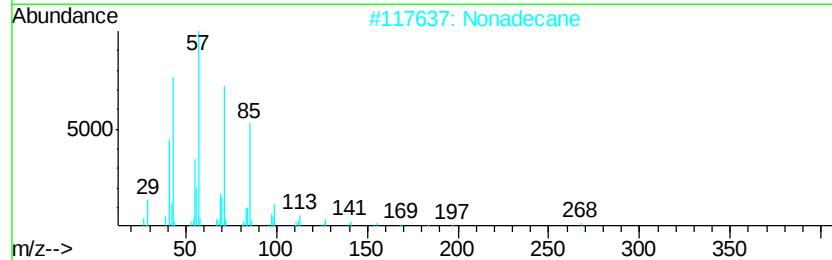
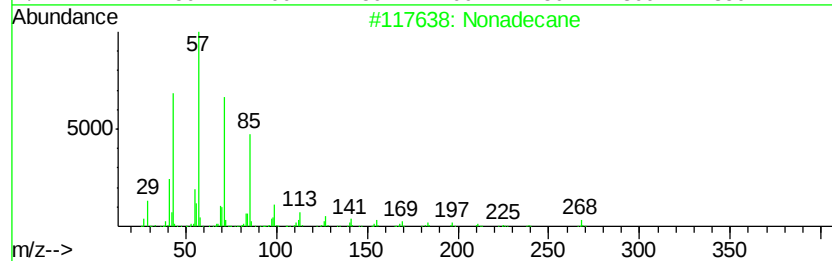
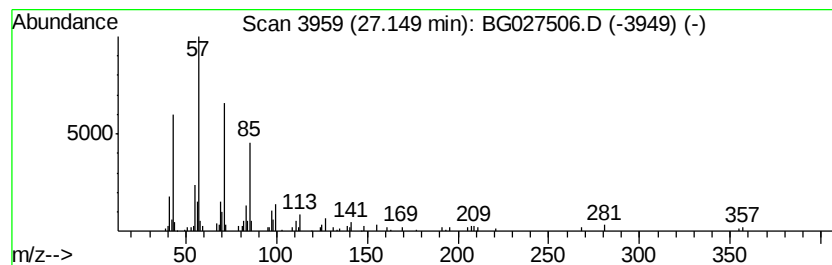
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.15	2.55 ng/ul	153013	Perylene-d12	25.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	95
2		Nonadecane	268	C19H40	000629-92-5	93
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027506.D
Acq On : 17 Jun 2017 13:52
Operator : SJ/MA
Sample : I3599-20
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5D38

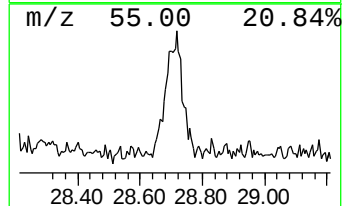
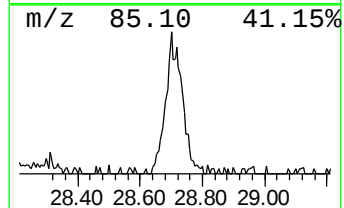
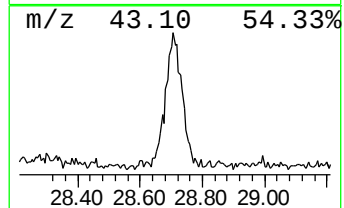
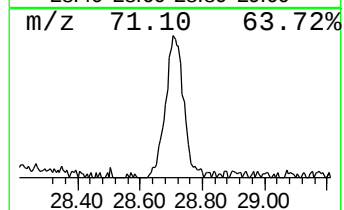
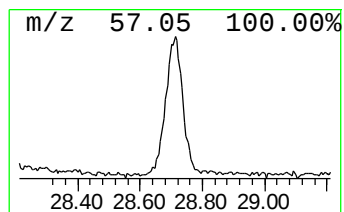
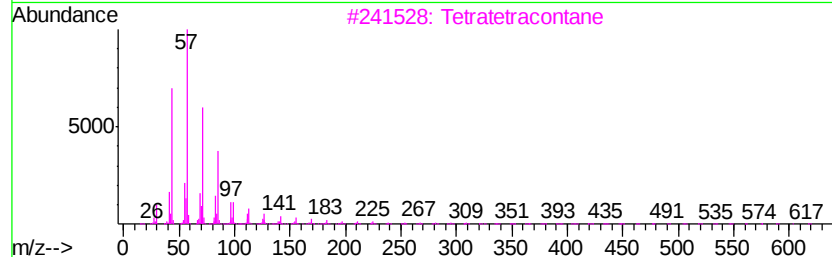
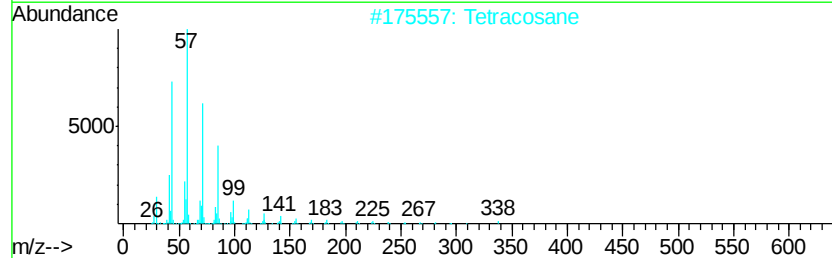
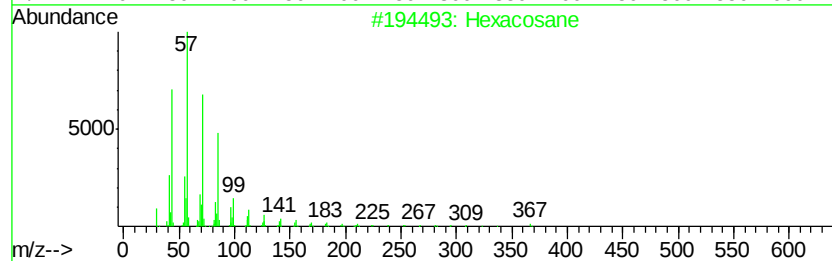
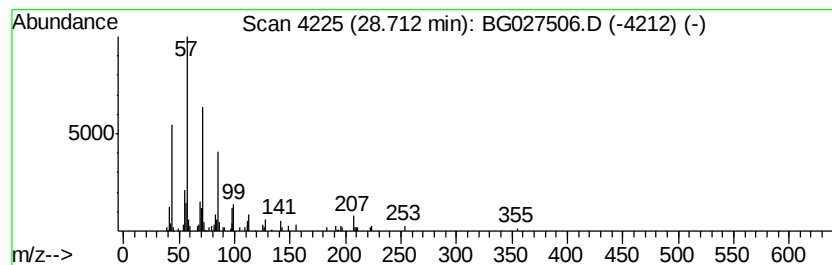
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.71	2.75 ng/ul	164699	Perylene-d12	25.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	87
2		Tetracosane	338	C24H50	000646-31-1	87
3		Tetratetracontane	619	C44H90	007098-22-8	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027506.D
Acq On : 17 Jun 2017 13:52
Operator : SJ/MA
Sample : I3599-20
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5D38

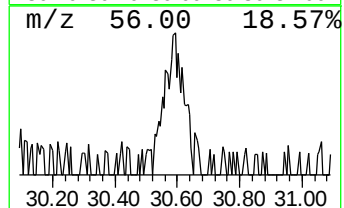
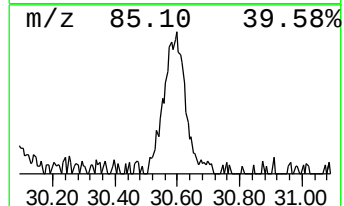
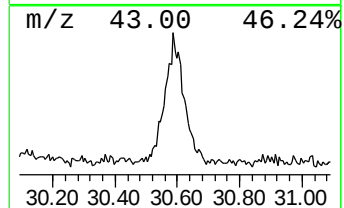
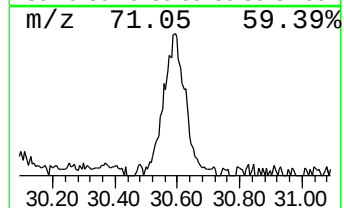
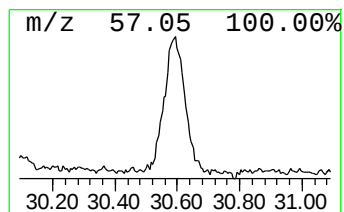
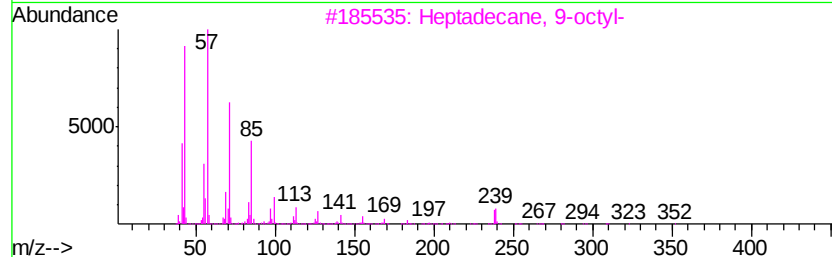
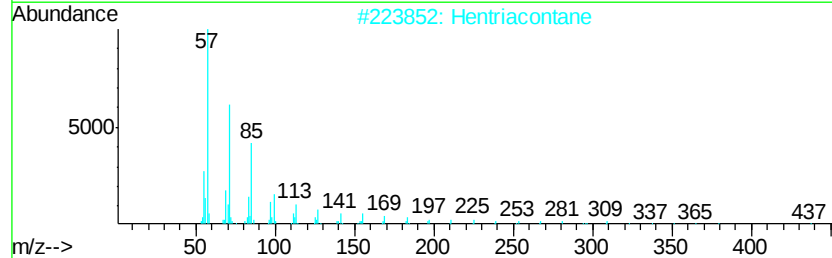
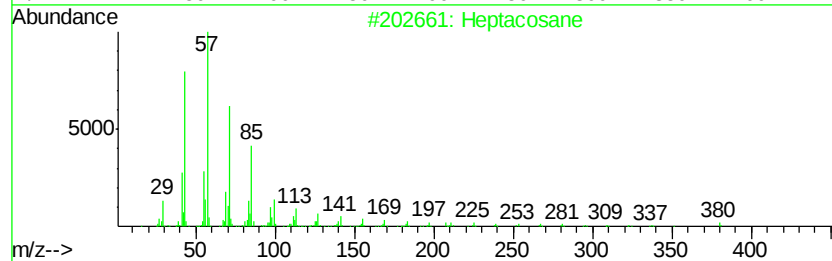
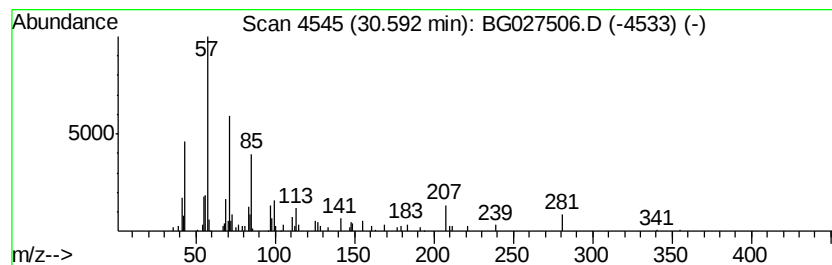
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.59	2.35 ng/ul	141160	Perylene-d12	25.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	80
2		Hentriacontane	437	C31H64	000630-04-6	80
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
4		10-Methylnonadecane	282	C20H42	056862-62-5	74
5		Hexacosane	366	C26H54	000630-01-3	74



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061617\
Data File : BG027506.D
Acq On : 17 Jun 2017 13:52
Operator : SJ/MA
Sample : I3599-20
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5D38

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG061617.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	18.69	3.5	ng/ul	169262	4	17.85	952838	20.0
unknown-01	20.53	2.1	ng/ul	114802	5	22.23	1096850	20.0
Trifluoroacetic a...	21.78	2.6	ng/ul	144959	5	22.23	1096850	20.0
(DEL) Alkane: Str...	27.15	2.5	ng/ul	153013	6	25.89	1199600	20.0
(DEL) Alkane: Str...	28.71	2.8	ng/ul	164699	6	25.89	1199600	20.0
(DEL) Alkane: Str...	30.59	2.4	ng/ul	141160	6	25.89	1199600	20.0