

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
 Data File : BG028511.D
 Acq On : 26 Aug 2017 4:17
 Operator : SJ/JU
 Sample : I4885-14
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B0AT0

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	3.735	20	25	31	rVB6	5643	10608	0.61%	0.059%
2	3.817	35	39	45	rBV3	10301	19178	1.11%	0.107%
3	4.076	79	83	93	rBV	31222	57689	3.33%	0.322%
4	4.992	236	239	245	rBV6	2213	3928	0.23%	0.022%
5	5.351	296	300	307	rVB4	1626	3748	0.22%	0.021%
6	5.439	307	315	322	rBV5	5031	12022	0.69%	0.067%
7	5.550	328	334	336	rBV5	2638	3443	0.20%	0.019%
8	5.797	369	376	381	rBV4	2631	6738	0.39%	0.038%
9	6.402	473	479	485	rBV5	3908	6451	0.37%	0.036%
10	6.543	500	503	508	rVB2	2814	4951	0.29%	0.028%
11	6.626	512	517	520	rBV2	3417	7341	0.42%	0.041%
12	6.767	537	541	544	rBV3	1844	3089	0.18%	0.017%
13	6.972	570	576	581	rBV5	3989	7074	0.41%	0.039%
14	7.325	631	636	642	rBV5	5904	10591	0.61%	0.059%
15	7.489	657	664	680	rVB	234757	487393	28.13%	2.719%
16	7.654	685	692	702	rVB	158106	275532	15.90%	1.537%
17	7.871	722	729	744	rVV	224420	407289	23.51%	2.272%
18	7.983	744	748	752	rVB4	2504	3921	0.23%	0.022%
19	8.241	787	792	801	rBV5	4351	11386	0.66%	0.064%
20	8.335	801	808	818	rVB	122531	225074	12.99%	1.255%
21	8.535	837	842	844	rBV2	3121	4996	0.29%	0.028%
22	8.647	858	861	867	rVB7	2809	4113	0.24%	0.023%
23	8.958	910	914	919	rBV4	3411	5131	0.30%	0.029%
24	9.035	919	927	943	rVV	310046	555720	32.07%	3.100%
25	9.176	949	951	958	rVB3	2193	3566	0.21%	0.020%
26	9.434	989	995	997	rVB4	1896	2916	0.17%	0.016%
27	9.505	997	1007	1019	rBV	224857	427203	24.66%	2.383%
28	9.604	1019	1024	1034	rBV2	17267	38750	2.24%	0.216%
29	9.740	1043	1047	1054	rVB4	1985	4980	0.29%	0.028%
30	10.233	1123	1131	1144	rBV	200125	380166	21.94%	2.121%
31	10.456	1164	1169	1173	rBV4	2538	4372	0.25%	0.024%
32	10.774	1214	1223	1239	rBV2	302302	586528	33.85%	3.272%
33	10.903	1239	1245	1256	rVV4	9782	23738	1.37%	0.132%
34	11.156	1280	1288	1302	rVB2	184700	342155	19.75%	1.909%

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35	11.291	1302	1311	1323	rVV	192572	380101	21.94%	2.120%
36	11.432	1330	1335	1339	rBV4	2370	5014	0.29%	0.028%
37	12.131	1444	1454	1458	rBV5	3037	9771	0.56%	0.055%
38	12.307	1479	1484	1490	rBV4	5305	9987	0.58%	0.056%
39	12.419	1502	1503	1509	rBV3	2075	3678	0.21%	0.021%
40	12.713	1549	1553	1561	rVB5	5408	11908	0.69%	0.066%
41	12.789	1561	1566	1572	rBV5	2400	5266	0.30%	0.029%
42	13.012	1596	1604	1608	rBV2	2115	4442	0.26%	0.025%
43	13.218	1635	1639	1647	rBV4	3167	7091	0.41%	0.040%
44	13.300	1647	1653	1656	rBV4	3810	6034	0.35%	0.034%
45	13.441	1673	1677	1686	rBV4	2549	6259	0.36%	0.035%
46	13.535	1686	1693	1697	rBV4	4109	8321	0.48%	0.046%
47	13.600	1697	1704	1712	rVB6	8138	14892	0.86%	0.083%
48	13.735	1720	1727	1729	rBV3	3545	5315	0.31%	0.030%
49	13.817	1736	1741	1744	rBV2	2900	4271	0.25%	0.024%
50	14.035	1774	1778	1783	rBV3	1959	4936	0.28%	0.028%
51	14.340	1820	1830	1834	rBV	604674	920295	53.11%	5.133%
52	14.387	1834	1838	1846	rVV	399026	599796	34.62%	3.346%
53	14.446	1846	1848	1855	rVV4	3338	5165	0.30%	0.029%
54	14.557	1863	1867	1874	rBV4	2906	5503	0.32%	0.031%
55	14.646	1874	1882	1893	rVB	628620	1010830	58.34%	5.638%
56	14.804	1904	1909	1915	rVB2	7768	11309	0.65%	0.063%
57	14.951	1925	1934	1942	rBV2	296995	502658	29.01%	2.804%
58	15.145	1959	1967	1981	rBV2	184127	401521	23.17%	2.240%
59	15.298	1990	1993	1994	rBV3	2724	3165	0.18%	0.018%
60	15.415	2010	2013	2016	rBV5	4290	4752	0.27%	0.027%
61	15.474	2020	2023	2027	rBV5	2821	3837	0.22%	0.021%
62	15.545	2034	2035	2040	rBV3	2868	3651	0.21%	0.020%
63	15.703	2055	2062	2066	rBV4	9663	16011	0.92%	0.089%
64	15.744	2066	2069	2075	rVB	20407	27562	1.59%	0.154%
65	15.821	2079	2082	2084	rVB4	3114	3137	0.18%	0.017%
66	15.938	2093	2102	2115	rBV	866540	1335422	77.07%	7.449%
67	16.062	2115	2123	2130	rBV	262289	412693	23.82%	2.302%
68	16.173	2133	2142	2150	rVB9	11722	34404	1.99%	0.192%
69	16.302	2161	2164	2171	rVB5	5713	9902	0.57%	0.055%
70	16.373	2171	2176	2180	rBV5	4510	8168	0.47%	0.046%
71	16.467	2187	2192	2196	rBV7	2842	5637	0.33%	0.031%

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72	16.608	2211	2216	2228	rVV3	29514	57990	3.35%	0.323%
73	16.784	2242	2246	2247	rBV3	3056	3926	0.23%	0.022%
74	16.831	2251	2254	2258	rBV5	2910	5053	0.29%	0.028%
75	16.890	2259	2264	2267	rVB6	2457	5346	0.31%	0.030%
76	16.966	2271	2277	2279	rBV5	5443	8815	0.51%	0.049%
77	17.072	2291	2295	2299	rVB5	6064	8190	0.47%	0.046%
78	17.119	2299	2303	2307	rBV6	4204	6216	0.36%	0.035%
79	17.401	2348	2351	2355	rBV2	23273	26861	1.55%	0.150%
80	17.454	2358	2360	2363	rVB3	7252	6887	0.40%	0.038%
81	17.548	2373	2376	2379	rVB5	2733	3018	0.17%	0.017%
82	17.701	2394	2402	2412	rBV2	393543	646548	37.31%	3.606%
83	17.801	2412	2419	2428	rVV	913672	1472854	85.00%	8.216%
84	17.871	2428	2431	2438	rVB7	9701	17524	1.01%	0.098%
85	17.942	2440	2443	2447	rBV6	4042	5705	0.33%	0.032%
86	18.036	2453	2459	2460	rBV4	5898	8615	0.50%	0.048%
87	18.142	2473	2477	2483	rVB3	13547	20419	1.18%	0.114%
88	18.183	2483	2484	2487	rBV3	2610	3210	0.19%	0.018%
89	18.547	2541	2546	2562	rBV2	144868	254747	14.70%	1.421%
90	19.704	2737	2743	2746	rBV3	14808	29974	1.73%	0.167%
91	19.804	2756	2760	2773	rBV4	58521	99807	5.76%	0.557%
92	20.075	2798	2806	2817	rVB	1171190	1732699	100.00%	9.665%
93	21.596	3060	3065	3079	rBV4	59839	144548	8.34%	0.806%
94	22.025	3131	3138	3152	rVB	425758	801248	46.24%	4.469%
95	23.570	3397	3401	3411	rVB9	22720	42111	2.43%	0.235%
96	24.751	3599	3602	3609	rVB7	29249	58599	3.38%	0.327%
97	25.298	3683	3695	3716	rVB2	518697	1702478	98.26%	9.497%
98	25.533	3719	3735	3751	rVB2	214174	801640	46.27%	4.472%
99	26.702	3926	3934	3943	rVB5	31354	104114	6.01%	0.581%
100	28.165	4179	4183	4197	rVB7	26568	83768	4.83%	0.467%

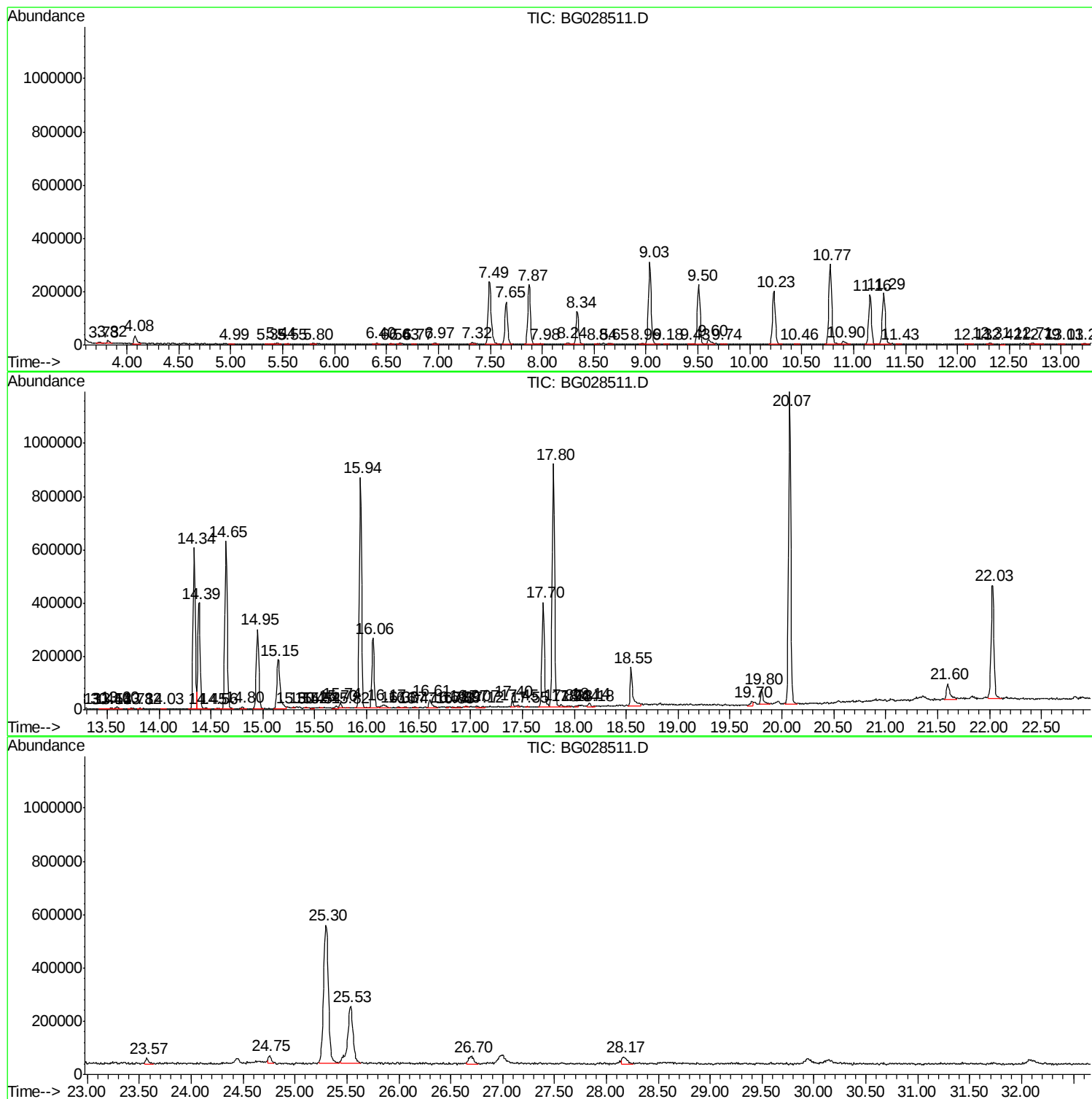
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Quant Title : SVOA CALIBRATION

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



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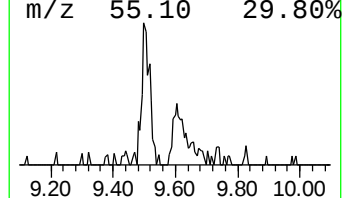
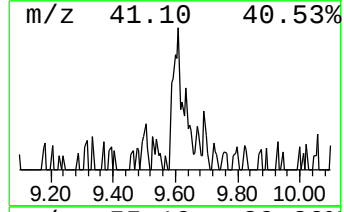
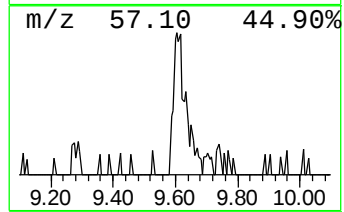
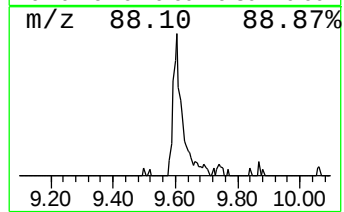
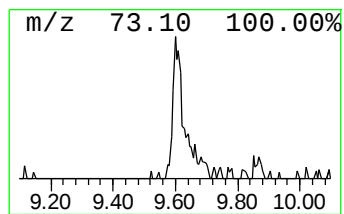
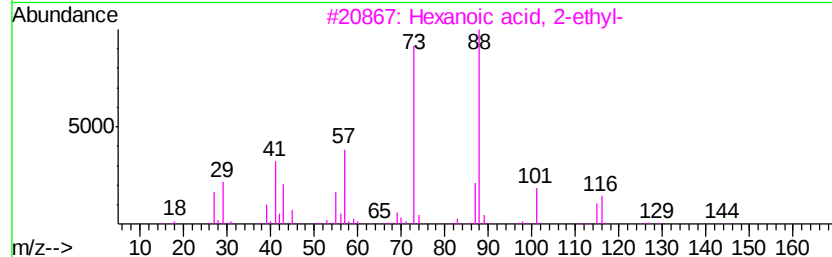
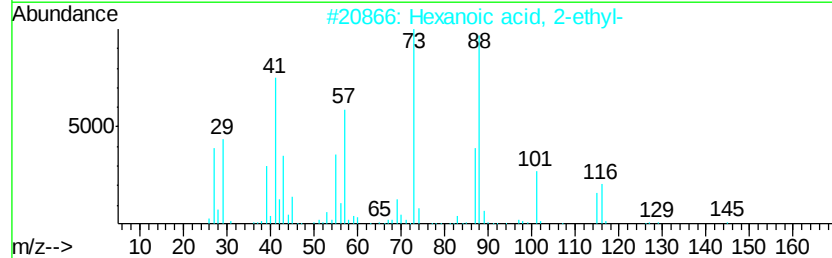
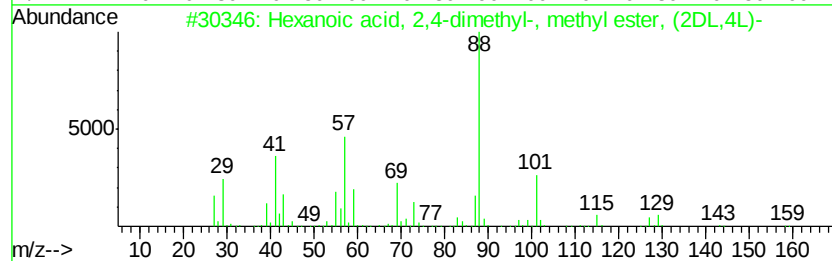
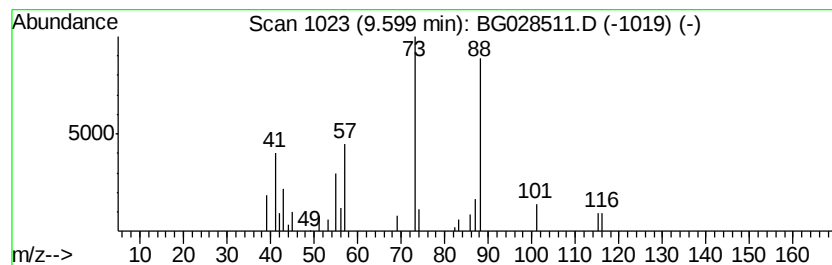
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexanoic acid, 2,4-dimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	3.44 ng/ul	38750	1,4-Dichlorobenzene-d4	8.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	59
2		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	50
3		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	45
4		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	45
5		Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	38



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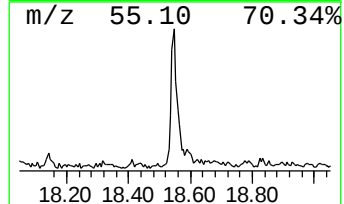
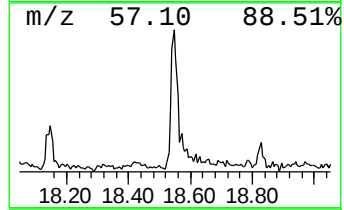
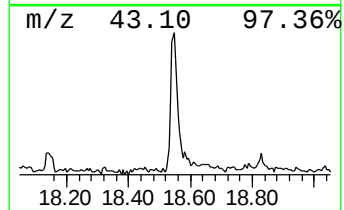
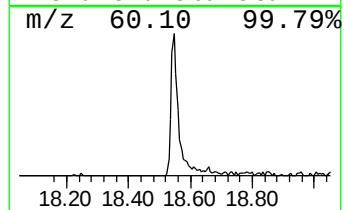
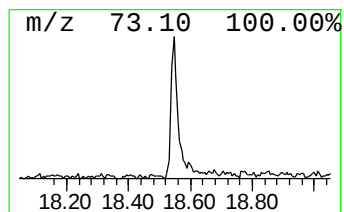
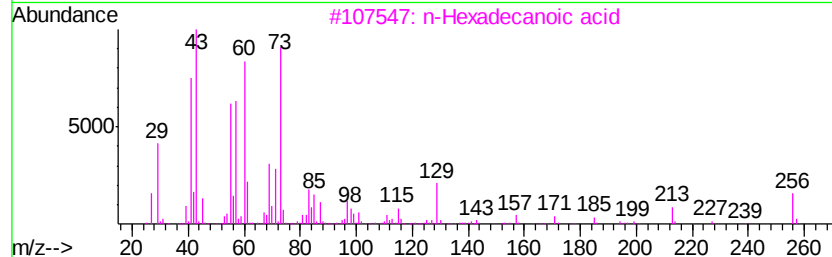
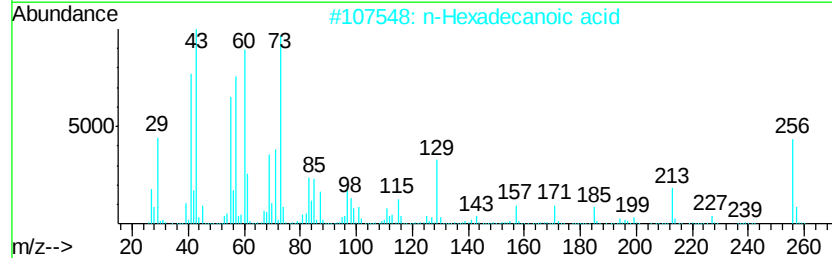
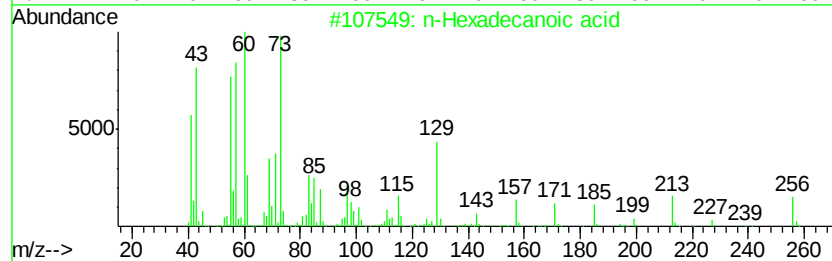
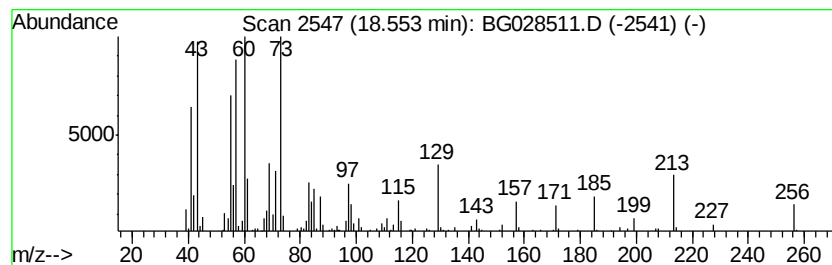
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	7.88 ng/ul	254747	Phenanthrene-d10	17.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
4		Tridecanoic acid	214	C13H26O2	000638-53-9	74
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	74



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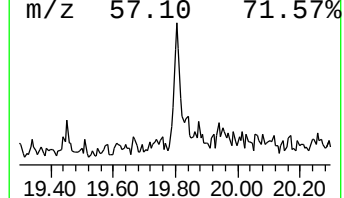
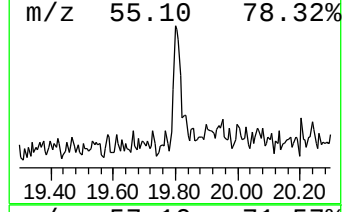
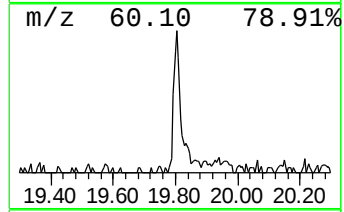
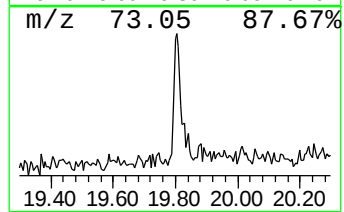
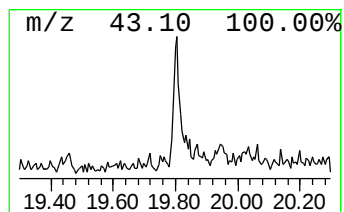
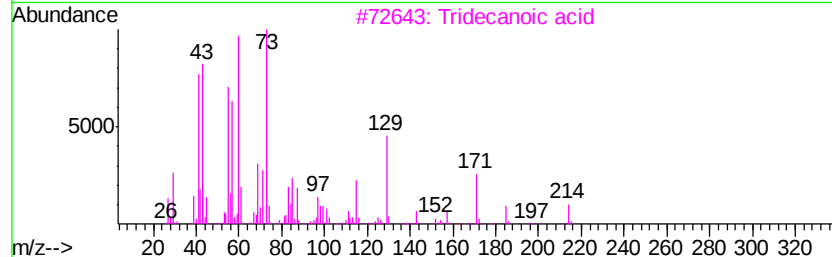
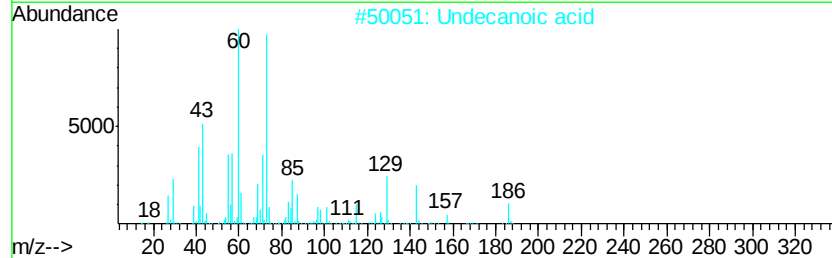
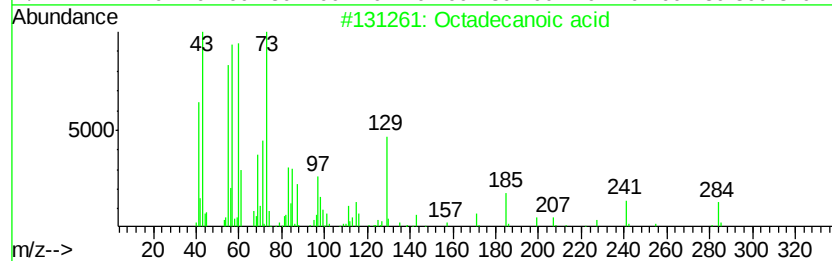
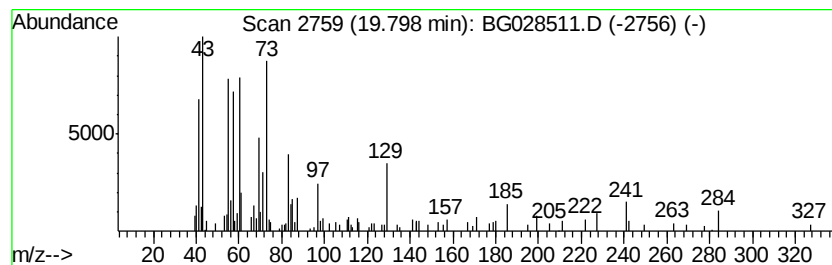
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.80	3.09 ng/ul	99807	Phenanthrene-d10	17.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Undecanoic acid	186	C11H22O2	000112-37-8	53
3		Tridecanoic acid	214	C13H26O2	000638-53-9	50
4		n-Decanoic acid	172	C10H20O2	000334-48-5	49
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
Data File : BG082511.D
Acq On : 26 Aug 2017 4:17
Operator : SJ/JU
Sample : I4885-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B0AT0

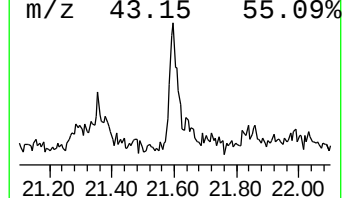
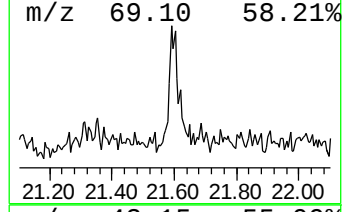
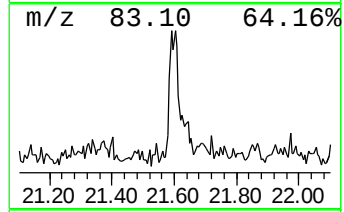
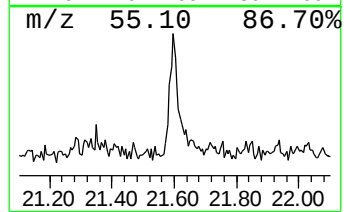
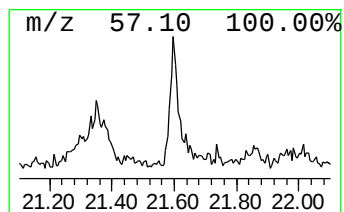
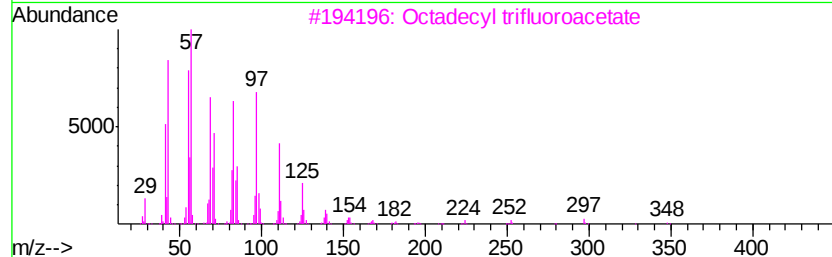
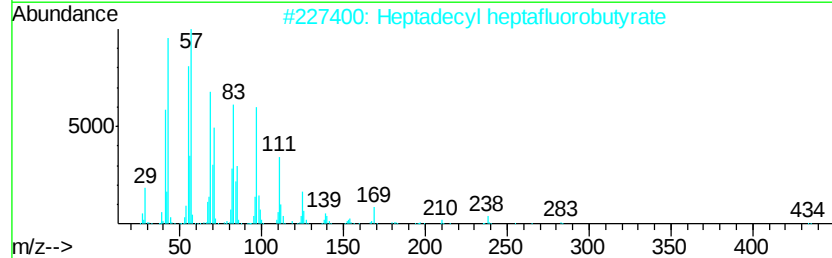
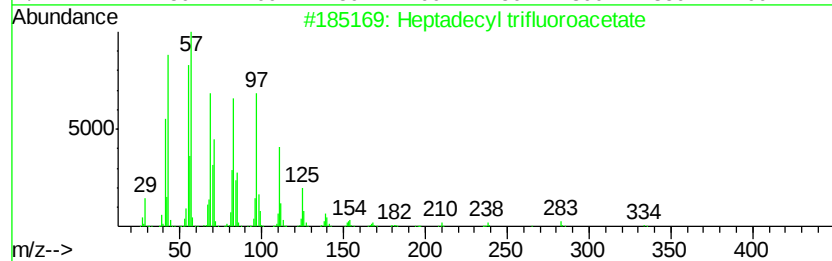
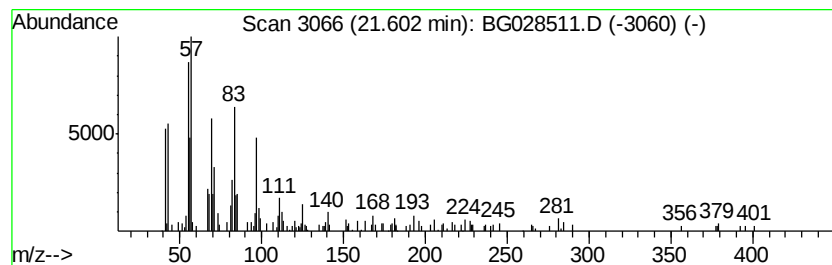
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.60	3.61 ng/ul	144548	Chrysene-d12	22.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
5		1-Docosene	308	C22H44	001599-67-3	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
Data File : BG082511.D
Acq On : 26 Aug 2017 4:17
Operator : SJ/JU
Sample : I4885-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B0AT0

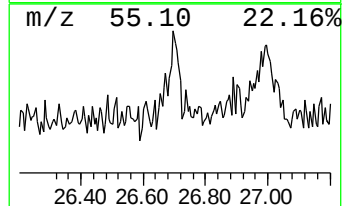
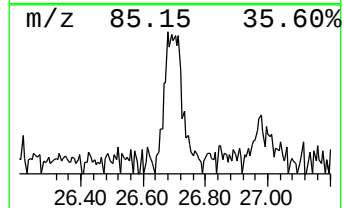
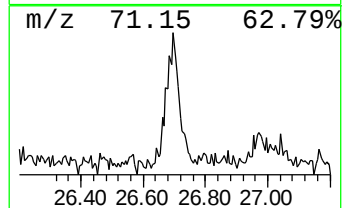
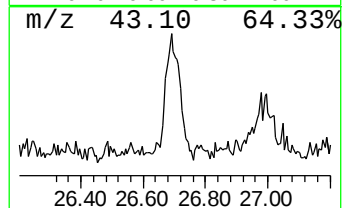
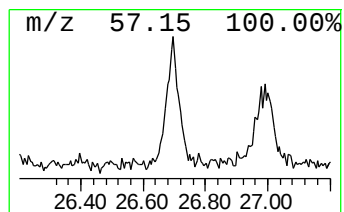
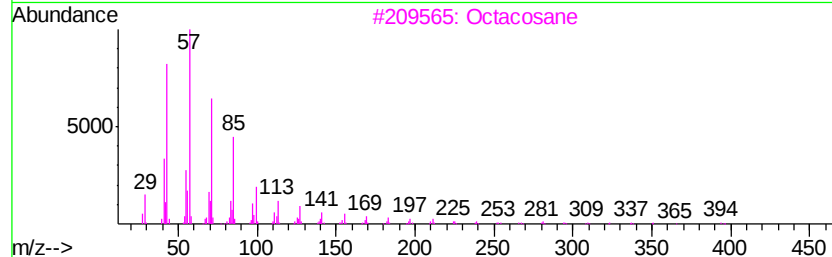
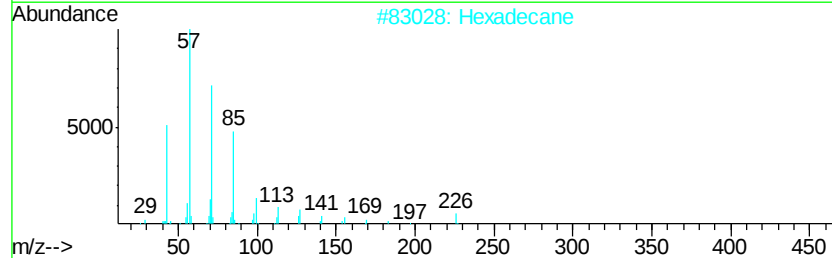
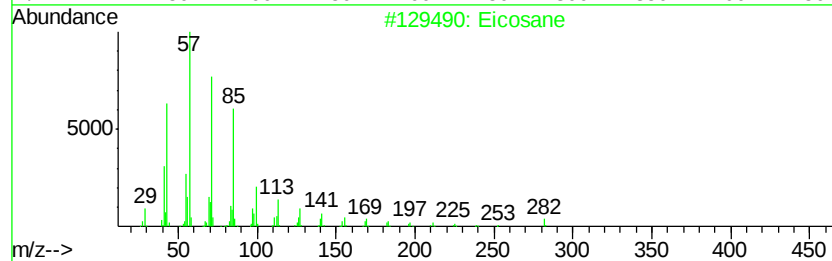
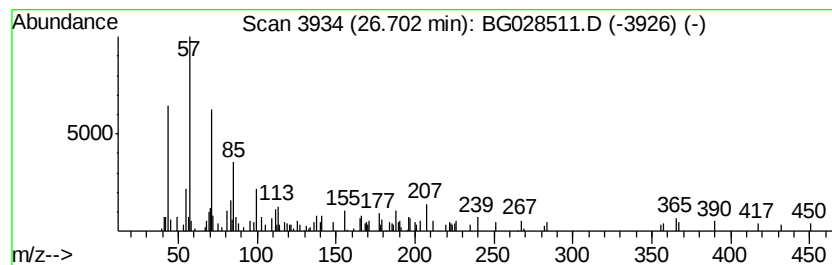
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.70	2.60 ng/ul	104114	Perylene-d12	25.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	55
2		Hexadecane	226	C16H34	000544-76-3	55
3		Octacosane	394	C28H58	000630-02-4	52
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	50
5		Hexacosane, 9-octyl-	479	C34H70	055429-83-9	49



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
Data File : BG082511.D
Acq On : 26 Aug 2017 4:17
Operator : SJ/JU
Sample : I4885-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B0AT0

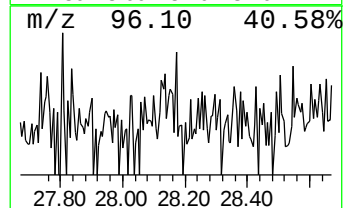
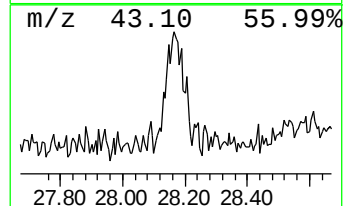
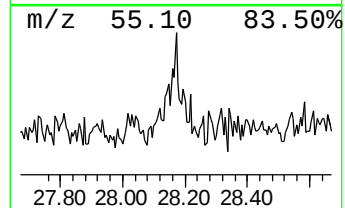
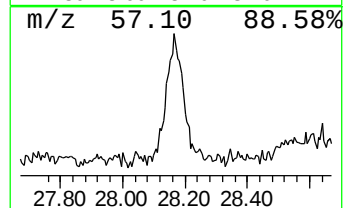
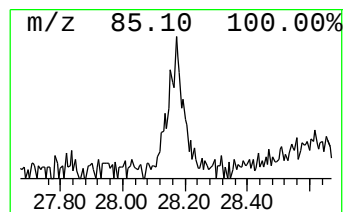
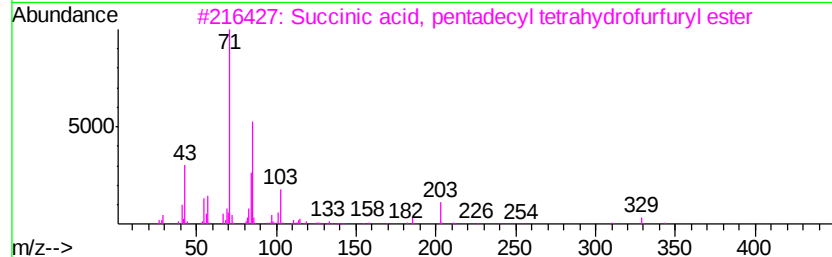
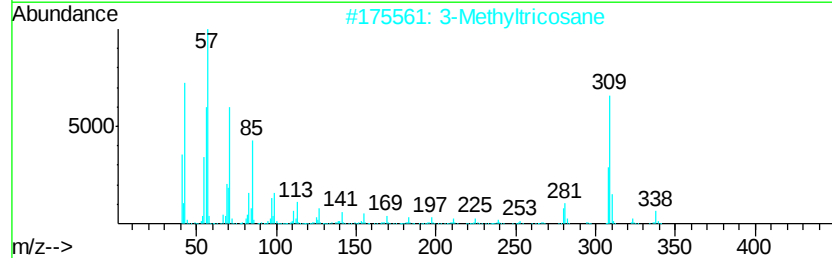
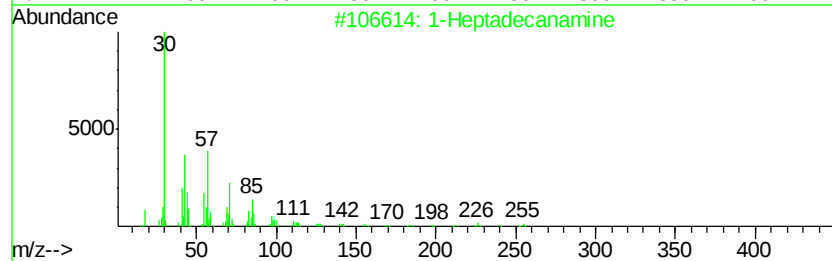
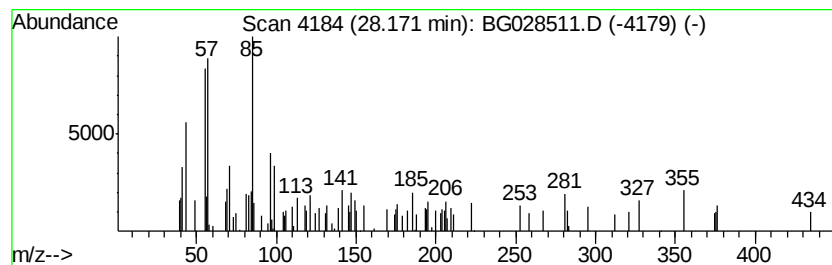
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG080217.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.17	2.09 ng/ul	83768	Perylene-d12	25.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptadecanamine	255	C17H37N	004200-95-7	32
2		3-Methyltricosane	338	C24H50	1000131-18-2	25
3		Succinic acid, pentadecyl tetrah...	412	C24H44O5	1000329-87-1	23
4		11-Methylhentriacontane	451	C32H66	035799-05-4	23
5		Succinic acid, heptadecyl tetrah...	440	C26H48O5	1000329-87-3	23



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG082517\
Data File : BG028511.D
Acq On : 26 Aug 2017 4:17
Operator : SJ/JU
Sample : I4885-14
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B0AT0

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
Hexanoic acid, 2,...	9.60	3.4	ng/ul	38750	1	8.34	225074	20.0
n-Hexadecanoic acid	18.55	7.9	ng/ul	254747	4	17.70	646548	20.0
Octadecanoic acid	19.80	3.1	ng/ul	99807	4	17.70	646548	20.0
Heptadecyl triflu...	21.60	3.6	ng/ul	144548	5	22.03	801248	20.0
(DEL) Alkane: Str...	26.70	2.6	ng/ul	104114	6	25.53	801640	20.0
unknown-01	28.17	2.1	ng/ul	83768	6	25.53	801640	20.0