

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
 Data File : BG021368.D
 Acq On : 8 Mar 2016 15:52
 Operator : UM/SJ
 Sample : H1655-13
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MS-DS-B350

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0.1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG030316.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	3.531	115	118	125	rVB	3006	4838	1.17%	0.110%
2	3.630	132	135	137	rBV2	460	569	0.14%	0.013%
3	4.453	272	275	278	rVB	465	553	0.13%	0.013%
4	4.999	365	368	373	rBV	389	638	0.15%	0.015%
5	5.370	428	431	433	rBB	588	568	0.14%	0.013%
6	6.521	626	627	633	rBV	358	599	0.15%	0.014%
7	7.273	749	755	764	rBV	72475	122785	29.75%	2.800%
8	7.444	778	784	794	rBB	54415	87310	21.15%	1.991%
9	7.655	813	820	827	rBV	69877	116576	28.24%	2.658%
10	8.125	893	900	907	rBB	42331	69992	16.96%	1.596%
11	8.818	1011	1018	1028	rBV	88842	151466	36.69%	3.453%
12	9.288	1091	1098	1106	rBV	72149	127476	30.88%	2.907%
13	9.377	1111	1113	1119	rVB	386	595	0.14%	0.014%
14	9.670	1160	1163	1167	rBB	706	903	0.22%	0.021%
15	10.011	1214	1221	1228	rBB	61962	110403	26.75%	2.517%
16	10.546	1306	1312	1320	rBB	84362	148600	36.00%	3.388%
17	10.934	1371	1378	1385	rBB	64794	111941	27.12%	2.552%
18	11.063	1393	1400	1408	rBV	83544	146468	35.48%	3.340%
19	12.508	1642	1646	1649	rBB2	982	1271	0.31%	0.029%
20	13.542	1820	1822	1825	rVB	1343	1416	0.34%	0.032%
21	13.613	1831	1834	1837	rBV	1590	1724	0.42%	0.039%
22	14.136	1916	1923	1927	rBV	149235	217239	52.63%	4.953%
23	14.177	1927	1930	1935	rVB	27072	35213	8.53%	0.803%
24	14.430	1966	1973	1980	rBV	169839	259106	62.77%	5.908%
25	14.606	1999	2003	2007	rBB	7550	9048	2.19%	0.206%
26	14.735	2017	2025	2032	rBB2	92862	144938	35.11%	3.305%
27	14.917	2049	2056	2064	rBV	83687	132988	32.22%	3.032%
28	15.041	2075	2077	2078	rBV	959	577	0.14%	0.013%
29	15.099	2085	2087	2092	rBV	1331	1644	0.40%	0.037%
30	15.164	2095	2098	2100	rBB2	1121	968	0.23%	0.022%
31	15.223	2104	2108	2112	rBB2	1739	2382	0.58%	0.054%
32	15.293	2115	2120	2122	rBV	1102	1186	0.29%	0.027%
33	15.505	2154	2156	2159	rBB	622	607	0.15%	0.014%
34	15.552	2159	2164	2169	rBB	11361	14226	3.45%	0.324%

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35	15.616	2170	2175	2177	rBV	1451	1287	0.31%	0.029%
36	15.722	2187	2193	2199	rBV	218205	319120	77.31%	7.276%
37	15.828	2206	2211	2218	rBB	75786	110139	26.68%	2.511%
38	15.963	2227	2234	2238	rBV3	4060	7278	1.76%	0.166%
39	15.998	2238	2240	2241	rVV3	972	631	0.15%	0.014%
40	16.057	2246	2250	2251	rBV	1741	1472	0.36%	0.034%
41	16.110	2254	2259	2266	rBB	1440	2303	0.56%	0.053%
42	16.180	2266	2271	2273	rBV2	1335	1847	0.45%	0.042%
43	16.251	2282	2283	2287	rBB2	540	543	0.13%	0.012%
44	16.415	2305	2311	2318	rBV	11361	19149	4.64%	0.437%
45	16.756	2364	2369	2372	rBV2	1138	2151	0.52%	0.049%
46	16.815	2377	2379	2382	rVV2	1268	1307	0.32%	0.030%
47	16.850	2382	2385	2387	rVV	1018	1452	0.35%	0.033%
48	16.874	2387	2389	2392	rVB	1067	835	0.20%	0.019%
49	16.921	2395	2397	2400	rVB	715	774	0.19%	0.018%
50	16.985	2405	2408	2411	rBB	933	831	0.20%	0.019%
51	17.203	2439	2445	2450	rBB3	4013	5535	1.34%	0.126%
52	17.261	2450	2455	2456	rBV	1217	1552	0.38%	0.035%
53	17.473	2484	2491	2498	rBB2	113939	172956	41.90%	3.943%
54	17.567	2501	2507	2514	rBV2	224386	348591	84.45%	7.948%
55	18.337	2633	2638	2645	rBV	23612	33830	8.20%	0.771%
56	18.419	2649	2652	2654	rVB3	928	1092	0.26%	0.025%
57	18.683	2693	2697	2701	rBV	438	554	0.13%	0.013%
58	19.277	2795	2798	2801	rVB	423	588	0.14%	0.013%
59	19.371	2810	2814	2815	rBV	501	542	0.13%	0.012%
60	19.482	2829	2833	2836	rBV2	2066	3064	0.74%	0.070%
61	19.518	2838	2839	2843	rVB2	747	802	0.19%	0.018%
62	19.559	2843	2846	2847	rBV	864	790	0.19%	0.018%
63	19.594	2849	2852	2858	rBV2	4181	5432	1.32%	0.124%
64	19.659	2861	2863	2868	rBV3	977	824	0.20%	0.019%
65	19.729	2871	2875	2877	rBV	1827	2230	0.54%	0.051%
66	19.841	2885	2894	2901	rBV	280791	412788	100.00%	9.412%
67	20.311	2972	2974	2975	rBV	809	561	0.14%	0.013%
68	20.728	3040	3045	3052	rBV2	10549	15024	3.64%	0.343%
69	20.963	3083	3085	3088	rVB2	2958	2978	0.72%	0.068%
70	21.351	3146	3151	3159	rBV4	25801	51062	12.37%	1.164%
71	21.727	3209	3215	3223	rBV	123765	200873	48.66%	4.580%

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72	23.196	3460	3465	3474	rVB4	15534	28697	6.95%	0.654%
73	23.401	3495	3500	3507	rVB2	20318	37384	9.06%	0.852%
74	24.759	3722	3731	3743	rVB	138977	370670	89.80%	8.451%
75	24.982	3760	3769	3778	rVB2	70925	189525	45.91%	4.321%

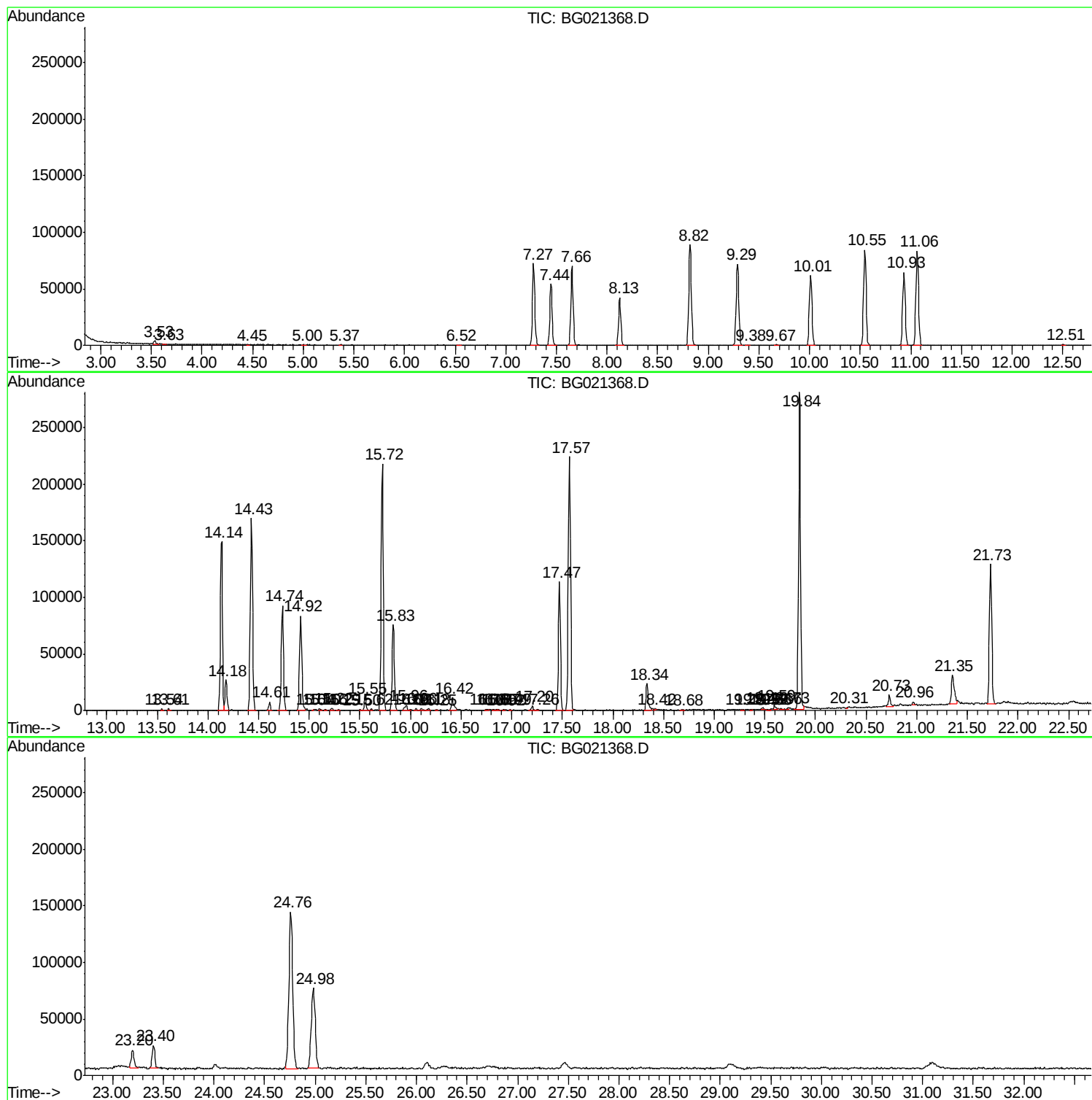
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG030316.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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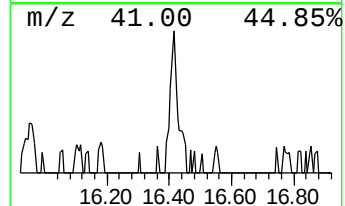
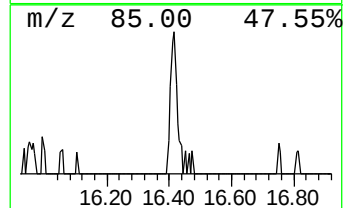
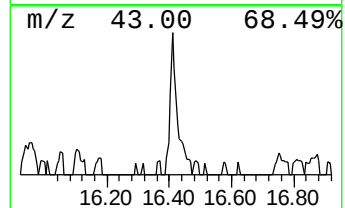
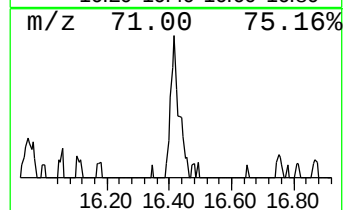
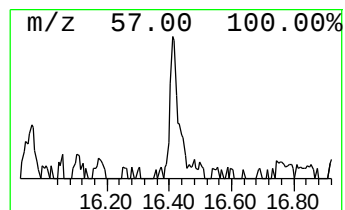
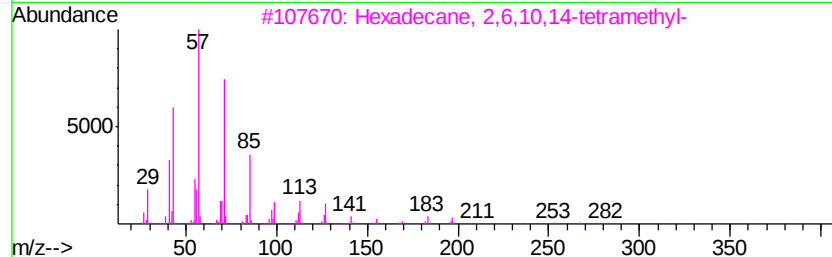
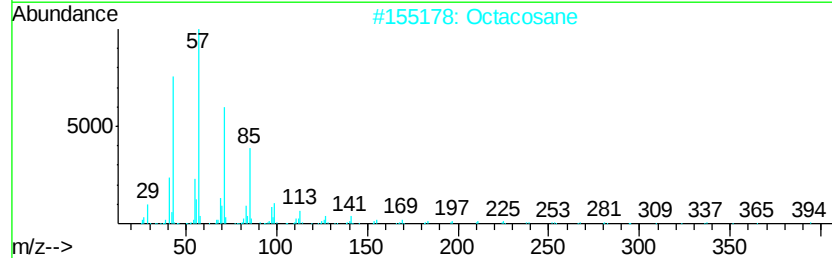
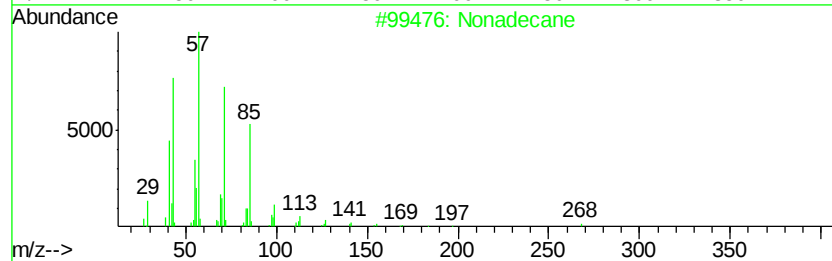
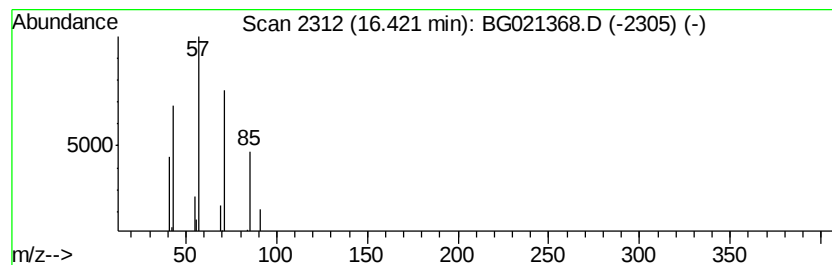
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG030316.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.42	2.21 ng/ul	19149	Phenanthrene-d10	17.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	90
2		Octacosane	394	C28H58	000630-02-4	83
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4		Eicosane	282	C20H42	000112-95-8	83
5		Heptadecane	240	C17H36	000629-78-7	83



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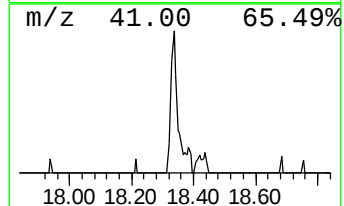
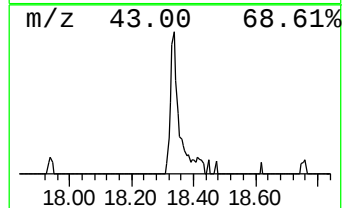
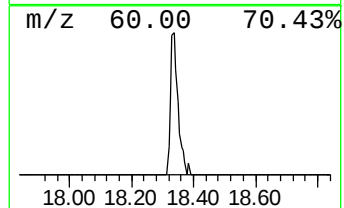
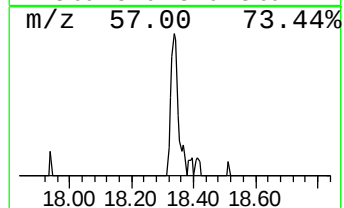
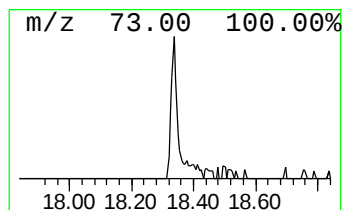
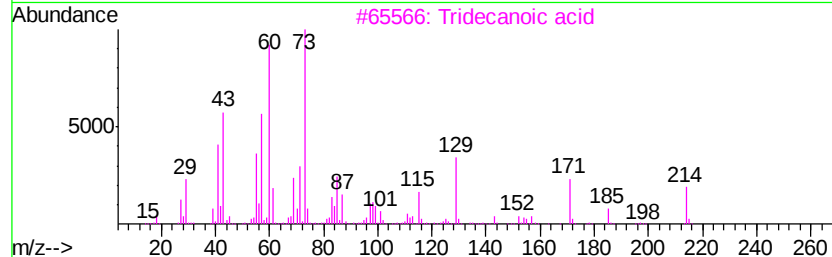
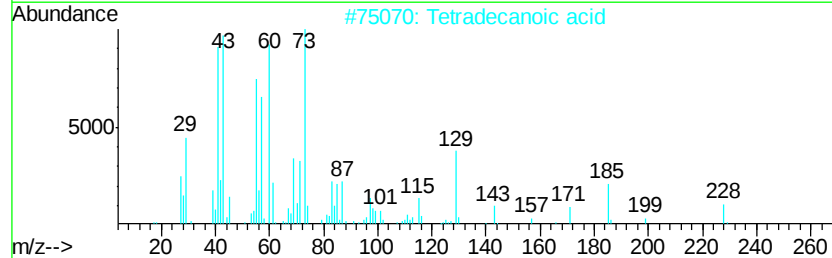
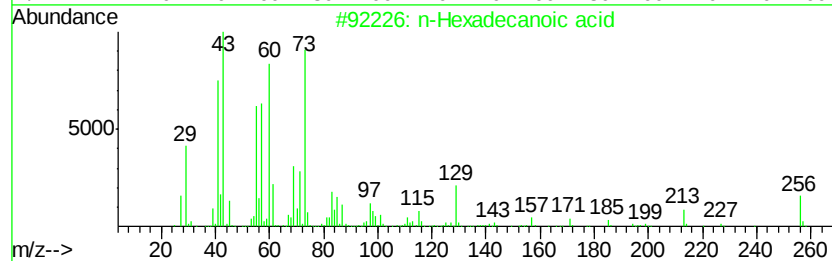
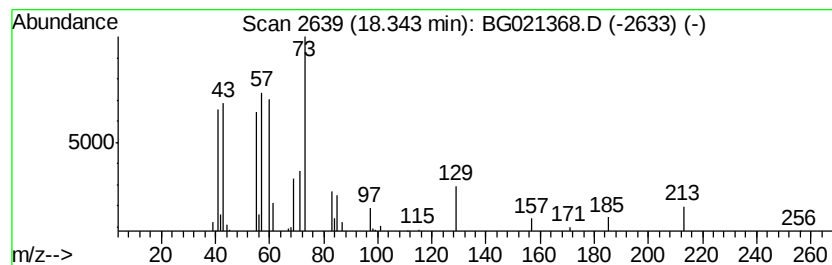
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	3.91 ng/ul	33830	Phenanthrene-d10	17.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3		Tridecanoic acid	214	C13H26O2	000638-53-9	43
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
5		Dodecanoic acid	200	C12H24O2	000143-07-7	43



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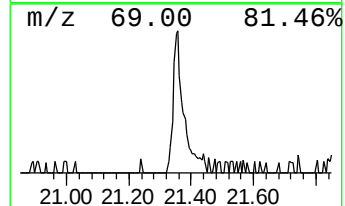
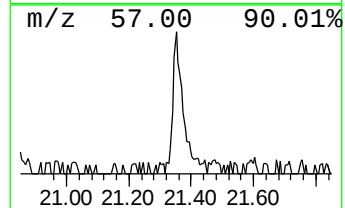
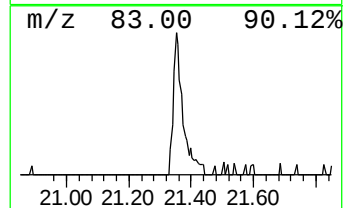
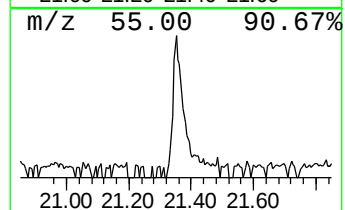
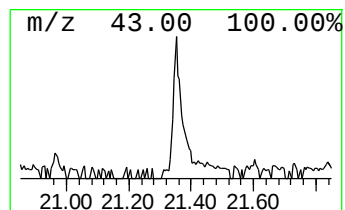
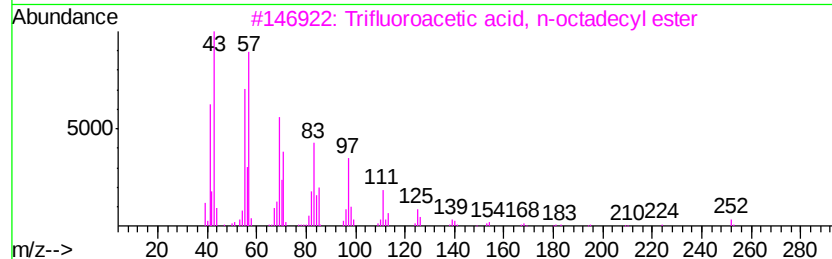
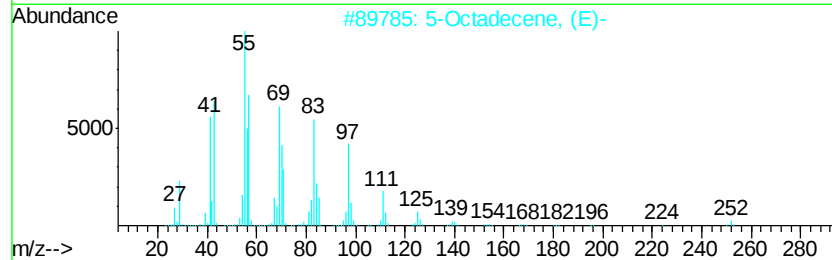
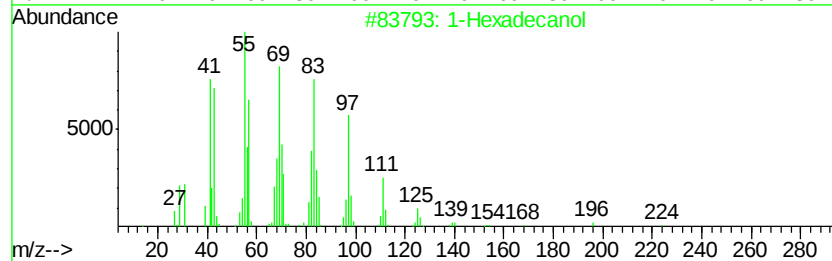
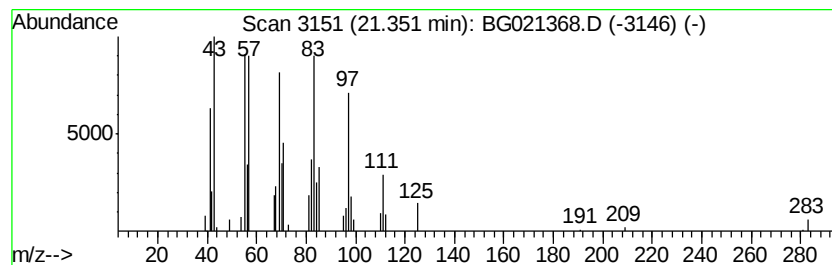
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 1-Hexadecanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	5.08 ng/ul	51062	Chrysene-d12	21.73
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4 87
2	5-Octadecene, (E)-	252	C18H36	007206-21-5 86
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1 83
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3 83
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1 83



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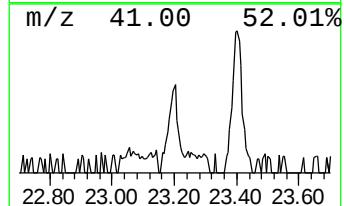
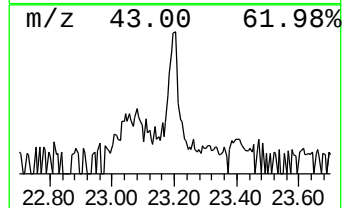
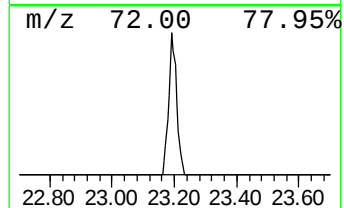
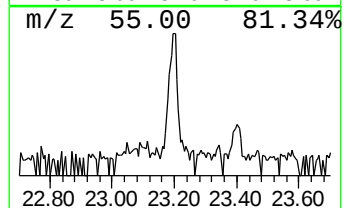
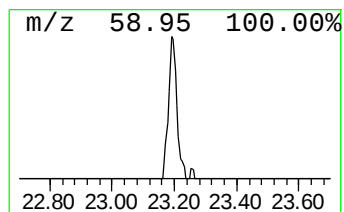
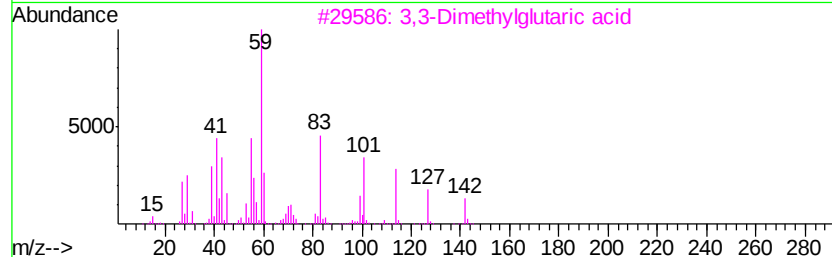
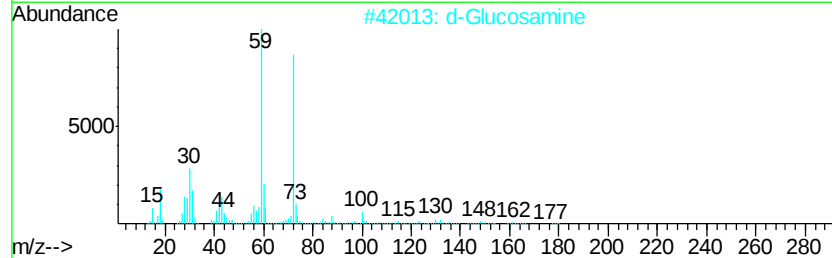
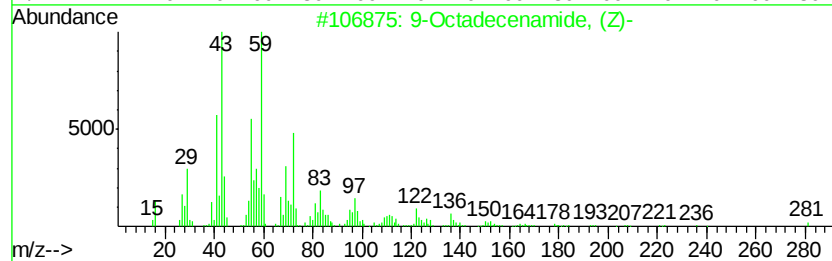
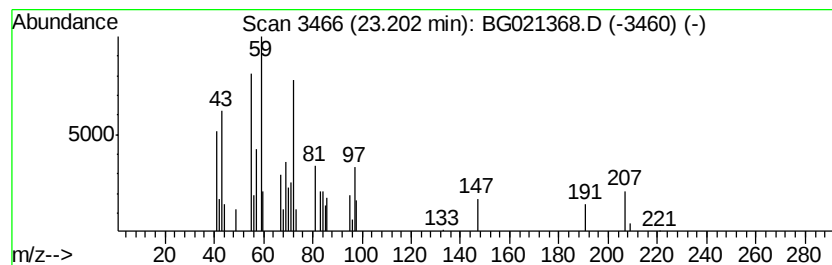
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.20	2.86 ng/ul	28697	Chrysene-d12	21.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	47
2		d-Glucosamine	179	C6H13NO5	000090-77-7	40
3		3,3-Dimethylglutaric acid	160	C7H12O4	004839-46-7	38
4		Methoxycarbonylsulphenyl chloride	126	C2H3ClO2S	026555-40-8	37
5		5-Carbamoyl-pentanoic acid ethyl...	173	C8H15NO3	001190-69-8	37



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021368.D
Acq On : 8 Mar 2016 15:52
Operator : UM/SJ
Sample : H1655-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MS-DS-B350

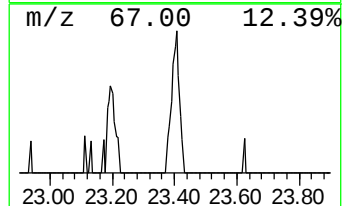
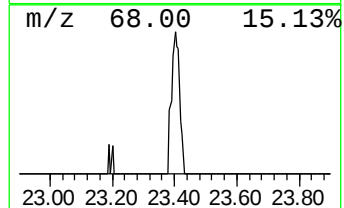
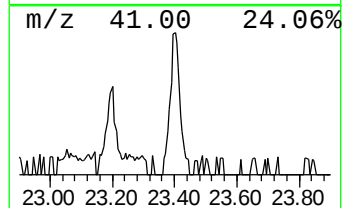
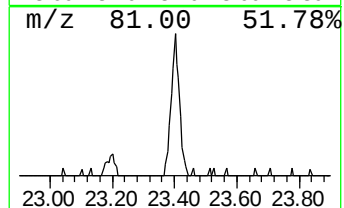
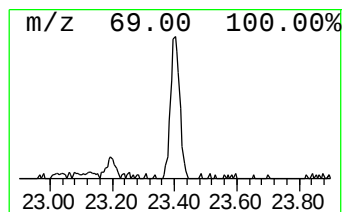
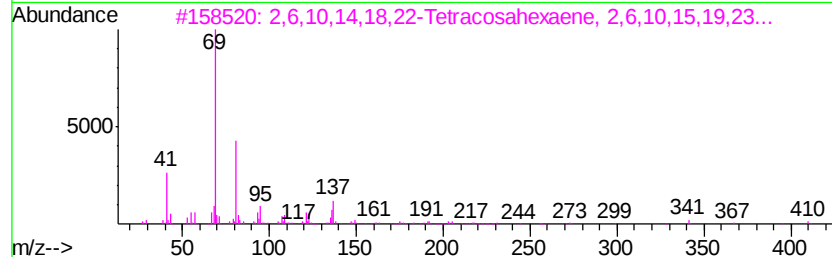
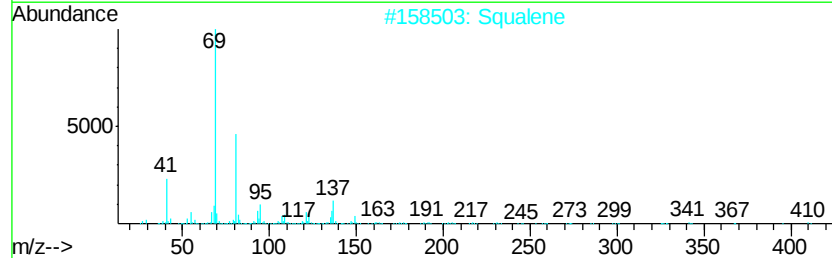
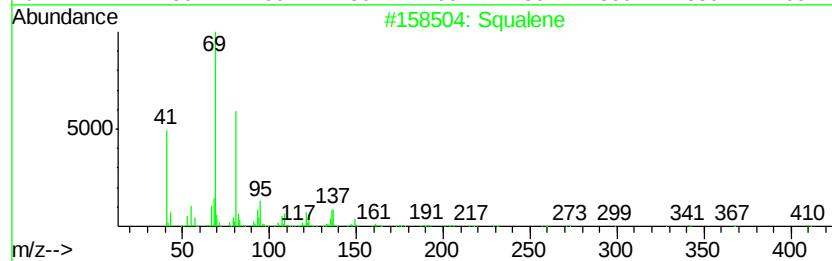
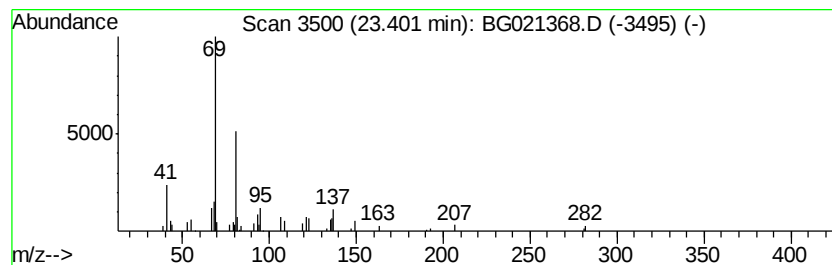
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	3.95 ng/ul	37384	Perylene-d12	24.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene		410	C30H50	007683-64-9	87
2	Squalene		410	C30H50	007683-64-9	86
3	2,6,10,14,18,22-Tetracosahexaene...		410	C30H50	000111-02-4	86
4	Docosa-2,6,10,14,18-pentaen-22-a...		384	C27H44O	1000163-04-7	72
5	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021368.D
Acq On : 8 Mar 2016 15:52
Operator : UM/SJ
Sample : H1655-13
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MS-DS-B350

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\SOM02.2-EPA-BG030316.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Str...	16.42	2.2	ng/ul	19149	4	17.47	172956	20.0
n-Hexadecanoic acid	18.34	3.9	ng/ul	33830	4	17.47	172956	20.0
1-Hexadecanol	21.35	5.1	ng/ul	51062	5	21.73	200873	20.0
unknown-01	23.20	2.9	ng/ul	28697	5	21.73	200873	20.0
Squalene	23.40	4.0	ng/ul	37384	6	24.98	189525	20.0