LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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:\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	3.188	56	59	63	rBV5	1132	1344	0.32%	0.028%
2	3.528	114	117	122	rBV	3298	4326	1.04%	0.091%
3	7.271	748	754	765	rBB	75305	126158	30.34%	2.654%
4	7.447	778	784	793	rBB	53870	90176	21.68%	1.897%
5	7.653	812	819	827	rBB	73588	121204	29.15%	2.550%
6	8.123	893	899	905	rBB2	43949	70364	16.92%	1.481%
7	8.816	1010	1017	1027	rBB	92483	156114	37.54%	3.285%
8	9.286	1090	1097	1104	rBV	73286	129996	31.26%	2.735%
9	10.009	1214	1220	1228	rBB	66043	114386	27.51%	2.407%
10	10.544	1303	1311	1319	rBB	89035	153252	36.85%	3.225%
11	10.932	1370	1377	1385	rBB	64291	112591	27.07%	2.369%
12	11.061	1392	1399	1412	rBB	84440	150512	36.19%	3.167%
13	13.540	1819	1821	1824	rBB	1664	1609	0.39%	0.034%
14	13.611	1830	1833	1837	rBB	1018	1348	0.32%	0.028%
15	14.134	1916	1922	1926	rBV	161501	225818	54.30%	4.751%
16	14.181	1926	1930	1935	rVV	20189	28613	6.88%	0.602%
17	14.427	1965	1972	1980	rBB	185270	274550	66.02%	5.777%
18	14.604	1998	2002	2006	rBB2	7222	8855	2.13%	0.186%
19	14.733	2017	2024	2032	rBB2	94840	147037	35.36%	3.094%
20	14.915	2048	2055	2063	rBV	86091	137808	33.14%	2.900%
21	15.056	2077	2079	2083	rVB2	1139	1379	0.33%	0.029%
22	15.097	2083	2086	2090	rBB	930	1120	0.27%	0.024%
23	15.156	2093	2096	2100	rBB	1195	1274	0.31%	0.027%
24	15.215	2104	2106	2111	rVV2	1869	2151	0.52%	0.045%
25	15.285	2115	2118	2123	rBB	978	1120	0.27%	0.024%
26	15.555	2159	2164	2171	rVB	11058	14053	3.38%	0.296%
27	15.608	2171	2173	2177	rBB2	1114	1439	0.35%	0.030%
28	15.720	2186	2192	2200	rBB	225112	336675	80.96%	7.084%
29	15.832	2205	2211	2221	rVV	80113	117025	28.14%	2.462%
30	15.955	2225	2232	2236	rBV3	4192	7732	1.86%	0.163%
31	16.049	2246	2248	2251	rVB2	1323	1325	0.32%	0.028%
32	16.108	2254	2258	2264	rBB	1371	1896	0.46%	0.040%
33	16.172	2266	2269	2274	rVB2	1592	1861	0.45%	0.039%
34	16.413	2305	2310	2317	rBV	10733	17814	4.28%	0.375%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

35	16.460	2317	2318	2321	rVV2	1258	1176	0.28%	0.025%
36	16.754	2366	2368	2371	rVV2	1383	1612	0.39%	0.034%
37	16.813	2375	2378	2382	rVV	1036	1286	0.31%	0.027%
38	17.201	2440	2444	2448	rBV	4395	6014	1.45%	0.127%
39	17.248	2450	2452	2458	rBB2	1351	1892	0.45%	0.040%
40	17.471	2484	2490	2497	rVV	118105	175545	42.21%	3.694%
41	17.565	2500	2506	2513	rVV2	237912	368608	88.64%	7.756%
42	18.335	2633	2637	2644	rBV2	15769	21796	5.24%	0.459%
43	19.198	2780	2784	2789	rBV2	1211	2135	0.51%	0.045%
44	19.474	2828	2831	2836	rVB2	1945	2641	0.64%	0.056%
45	19.598	2848	2852	2857	rVB2	2763	4688	1.13%	0.099%
46	19.733	2869	2875	2878	rVV	1254	2217	0.53%	0.047%
47	19.839	2887	2893	2905	rBV	280737	415864	100.00%	8.750%
48	20.027	2920	2925	2927	rVB2	993	1417	0.34%	0.030%
49	20.080	2932	2934	2940	rVB3	632	1072	0.26%	0.023%
50	20.315	2973	2974	2975	rBV	1848	1156	0.28%	0.024%
51	20.579	3016	3019	3022	rBV4	1509	1806	0.43%	0.038%
52	20.773	3050	3052	3056	rBV4	1108	1406	0.34%	0.030%
53	20.832	3059	3062	3063	rBV4	2384	2310	0.56%	0.049%
54	20.885	3069	3071	3074	rVB2	954	1103	0.27%	0.023%
55	20.967	3082	3085	3088	rVB2	1540	1826	0.44%	0.038%
56	21.237	3129	3131	3132	rBV2	1592	1370	0.33%	0.029%
57	21.349	3145	3150	3163	rBV2	74799	140165	33.70%	2.949%
58	21.725	3208	3214	3222	rVB	126223	206657	49.69%	4.348%
59	21.789	3222	3225	3228	rBV4	1503	2071	0.50%	0.044%
60	21.866	3234	3238	3241	rVB4	2299	2499	0.60%	0.053%
61	21.989	3257	3259	3262	rBV3	1344	1430	0.34%	0.030%
62	22.183	3290	3292	3294	rBV3	1243	1061	0.26%	0.022%
63	22.406	3328	3330	3333	rVB4	1295	1439	0.35%	0.030%
64	22.518	3344	3349	3350	rBV4	3142	4366	1.05%	0.092%
65	22.547	3350	3354	3359	rVB7	2758	5794	1.39%	0.122%
66	22.782	3393	3394	3397	rBV2	1847	1515	0.36%	0.032%
67	22.823	3400	3401	3403	rBV2	1400	1107	0.27%	0.023%
68	22.941	3419	3421	3425	rBV4	1277	1636	0.39%	0.034%
69	23.023	3433	3435	3436	rBV2	1659	1421	0.34%	0.030%
70	23.082	3444	3445	3448	rBV2	1246	1075	0.26%	0.023%
71	23.194	3457	3464	3473	rBV4	36778	74800	17.99%	1.574%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

72	23.399	3494	3499	3509	rVB2	25163	48026	11.55%	1.011%
73	23.687	3546	3548	3550	rBV3	1125	1068	0.26%	0.022%
74	23.711	3550	3552	3555	rVB4	2257	1887	0.45%	0.040%
75	23.799	3565	3567	3569	rBV2	1320	1362	0.33%	0.029%
76	24.016	3597	3604	3610	rBV5	6270	14949	3.59%	0.315%
77	24.463	3678	3680	3681	rVB2	1832	1161	0.28%	0.024%
78	24.592	3701	3702	3705	rBV3	1949	1161	0.28%	0.024%
79	24.756	3719	3730	3743	rBV	145188	381634	91.77%	8.030%
80	24.980	3757	3768	3779	rBV3	74383	206555	49.67%	4.346%
81	26.096	3953	3958	3965	rVB7	6892	17245	4.15%	0.363%
82	26.225	3976	3980	3981	rBV3	3489	3770	0.91%	0.079%
83	27.130	4132	4134	4135	rBV2	1780	1179	0.28%	0.025%
84	27.377	4175	4176	4178	rBV2	1239	1156	0.28%	0.024%
85	27.459	4181	4190	4191	rBV8	7075	16153	3.88%	0.340%
86	27.659	4222	4224	4225	rBV2	1321	1031	0.25%	0.022%
87	27.970	4275	4277	4278	rVB2	2045	1099	0.26%	0.023%
88	28.000	4278	4282	4283	rBV4	1958	2014	0.48%	0.042%
89	28.529	4370	4372	4376	rBV5	1221	1352	0.33%	0.028%
90	28.787	4415	4416	4418	rBV2	1594	1141	0.27%	0.024%
91	29.057	4460	4462	4463	rBV2	1511	1098	0.26%	0.023%
92	29.974	4617	4618	4621	rBV3	1356	1097	0.26%	0.023%
93	30.291	4670	4672	4675	rVB4	1615	1420	0.34%	0.030%
94	30.326	4675	4678	4679	rBV3	1383	1637	0.39%	0.034%
95	30.779	4753	4755	4757	rBV3	1590	1180	0.28%	0.025%
96	31.084	4804	4807	4814	rVB8	3554	7526	1.81%	0.158%
97	31.454	4868	4870	4871	rBV2	1257	1093	0.26%	0.023%
98	31.713	4912	4914	4920	rVB4	1667	2200	0.53%	0.046%
99	32.459	5040	5041	5043	rBV	1532	1212	0.29%	0.026%
100	32.518	5049	5051	5053	rBV3	1389	1340	0.32%	0.028%

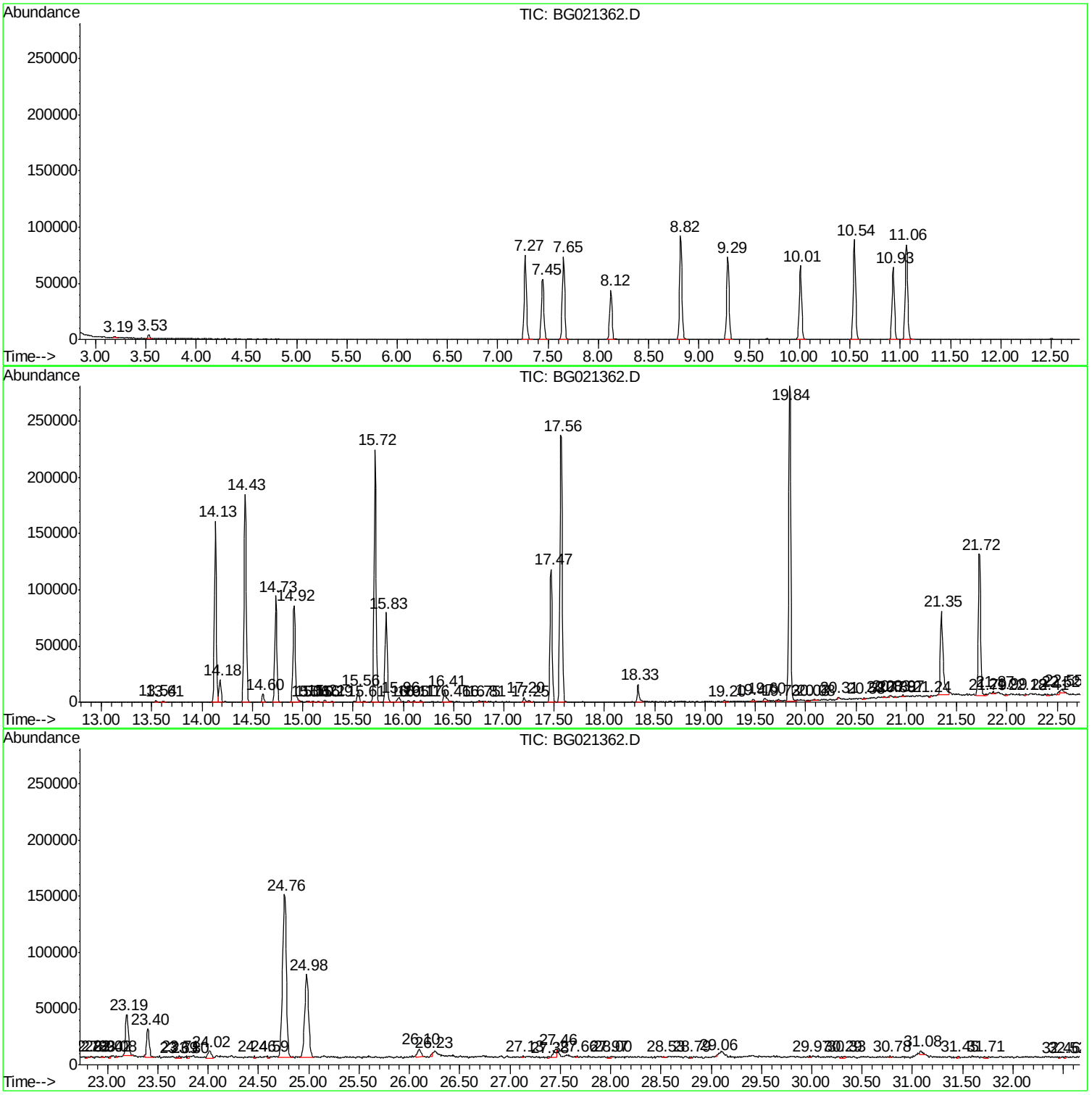
Sum of corrected areas: 4752647

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MS-DS-C70

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

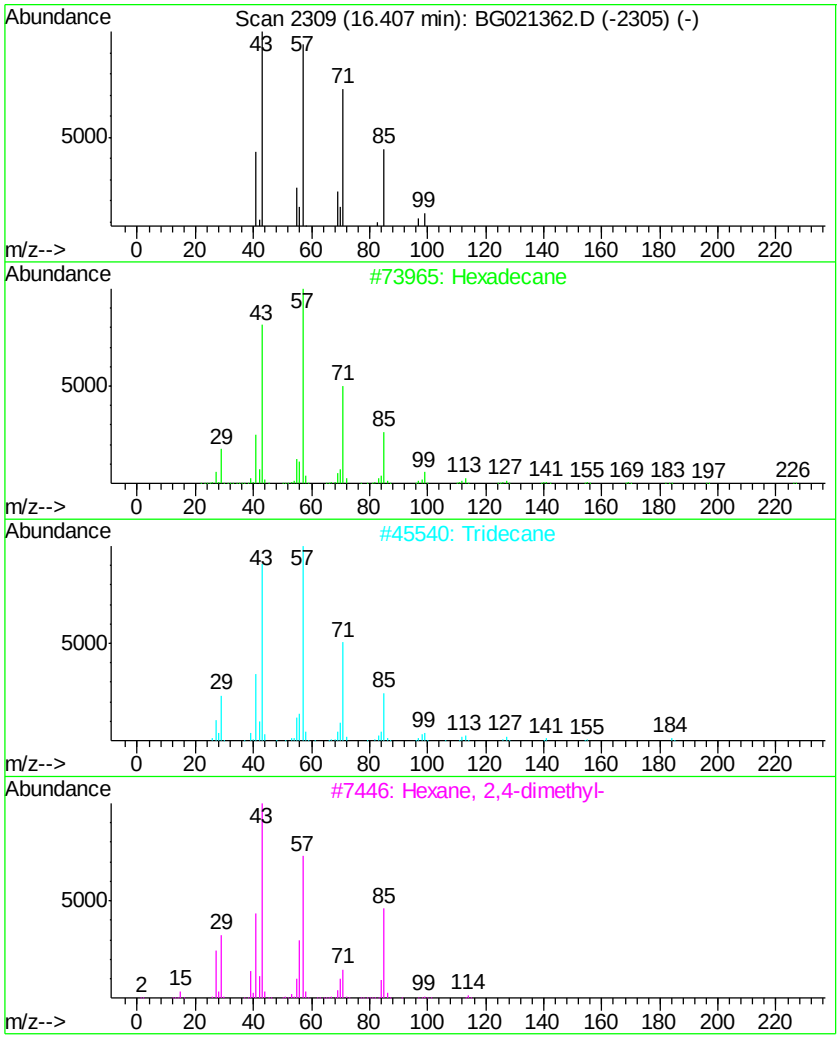
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

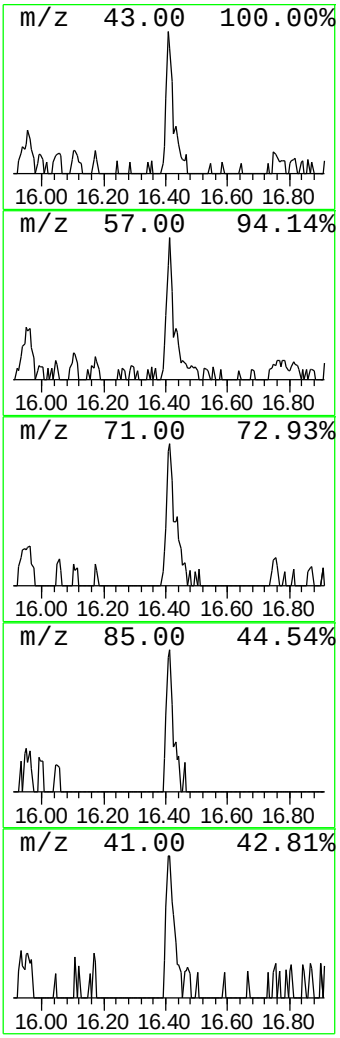
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	2.03 ng/ul	17814	Phenanthrene-d10	17.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	74
2	Tridecane	184	C13H28	000629-50-5	64
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	47
4	Nonane, 2,5-dimethyl-	156	C11H24	017302-27-1	42
5	Ether, hexyl pentyl	172	C11H24O	032357-83-8	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

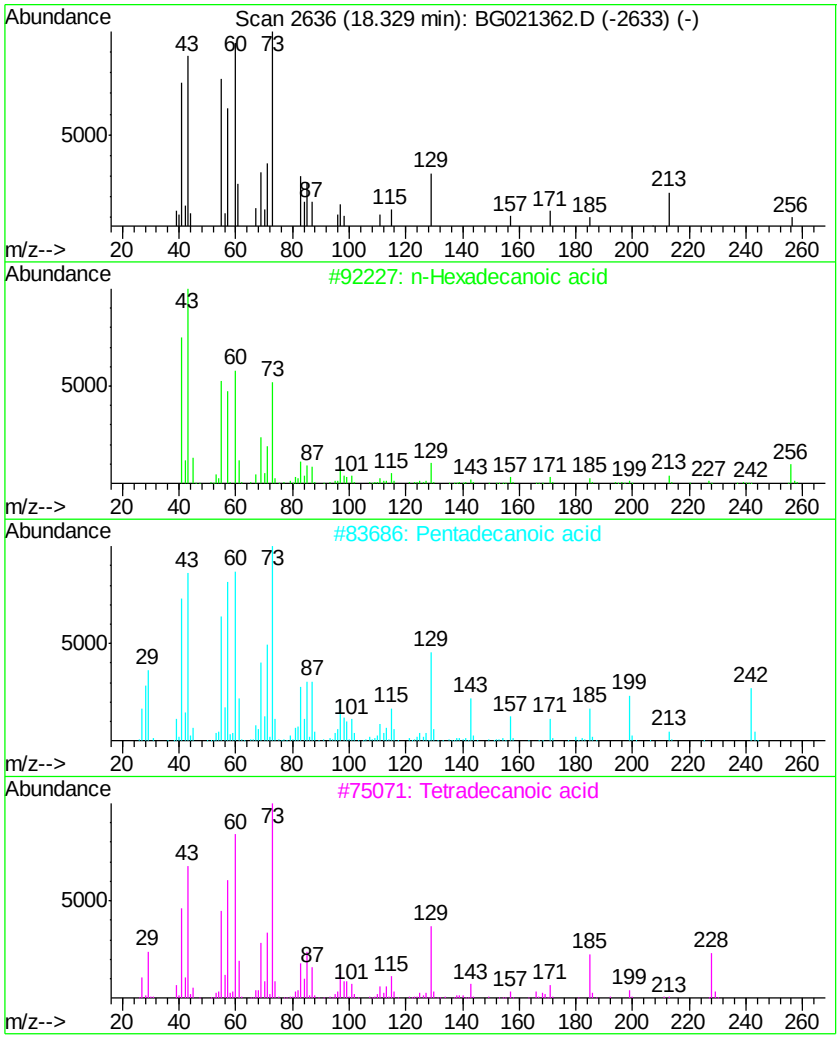
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

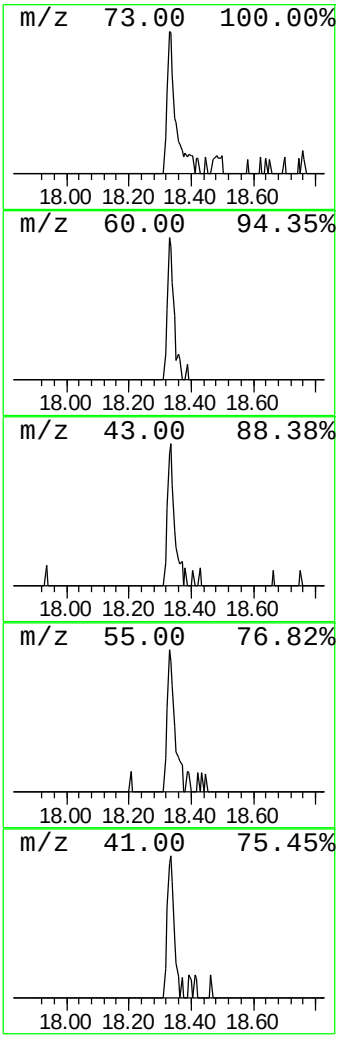
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.48 ng/ul	21796	Phenanthrene-d10	17.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

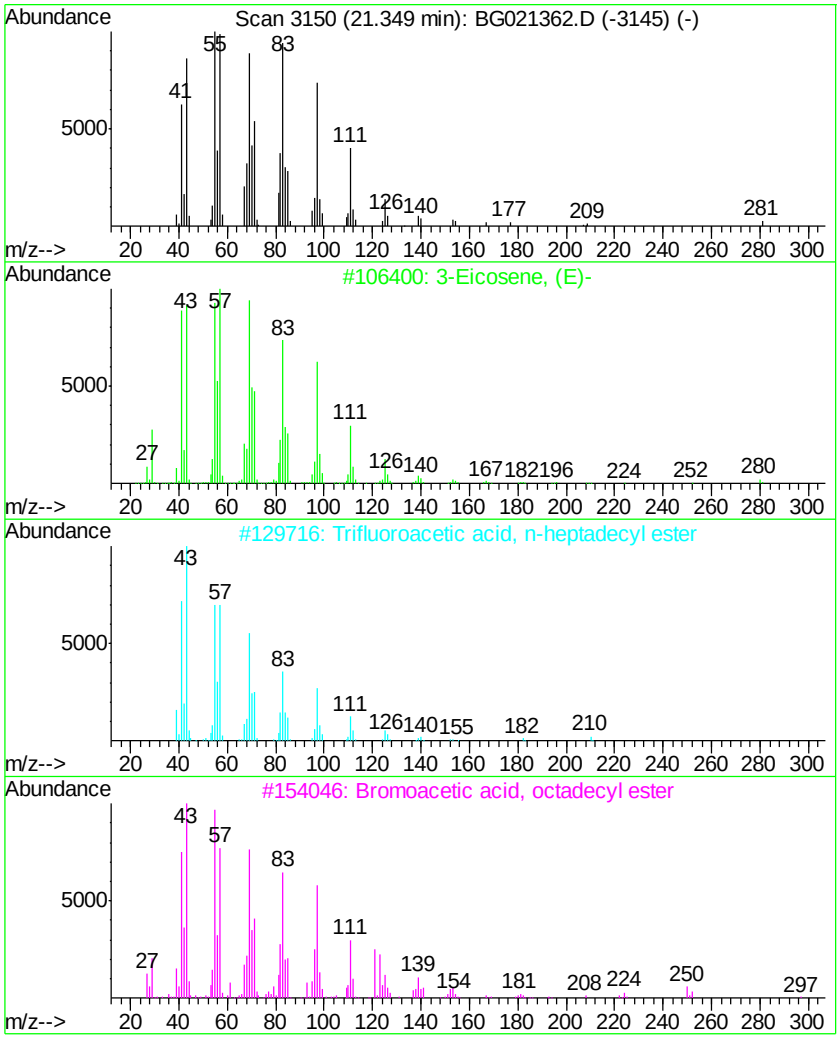
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

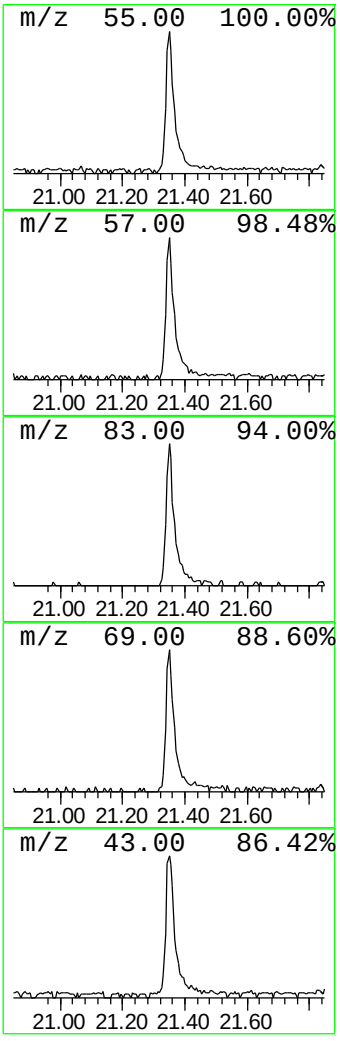
****

Peak Number 3 (DEL) Alkane: Cyclic21.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	13.57 ng/ul	140165	Chrysene-d12	21.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	90
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

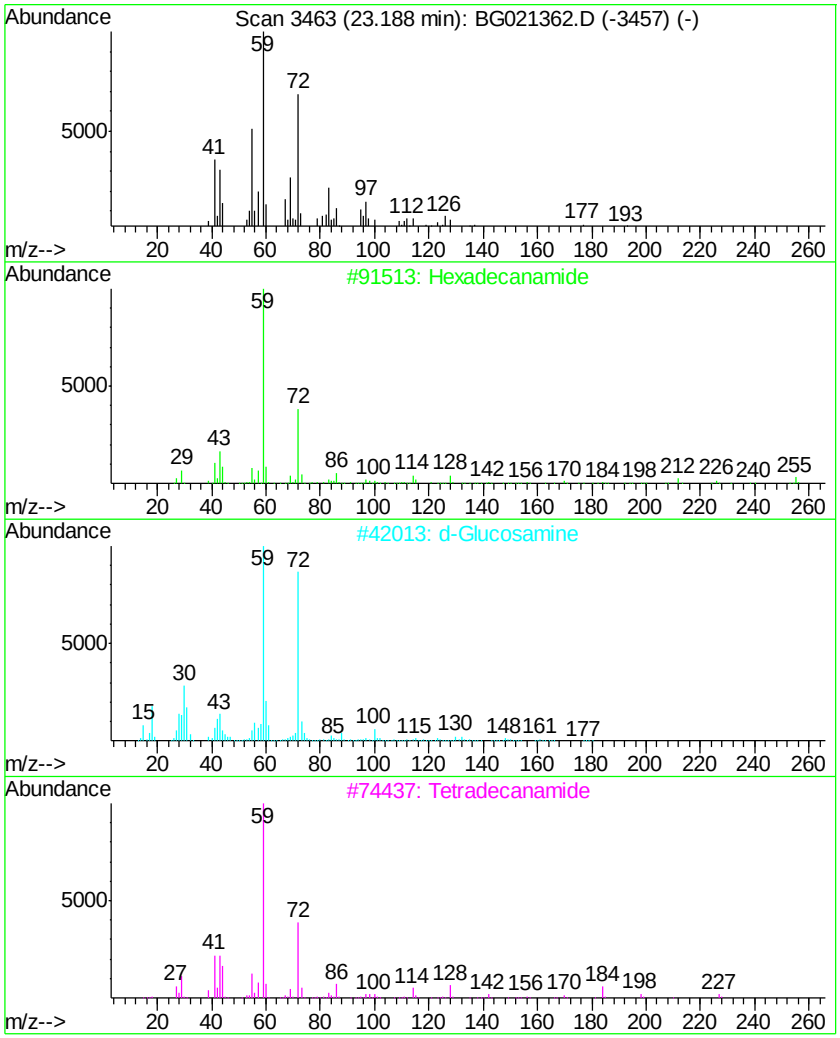
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

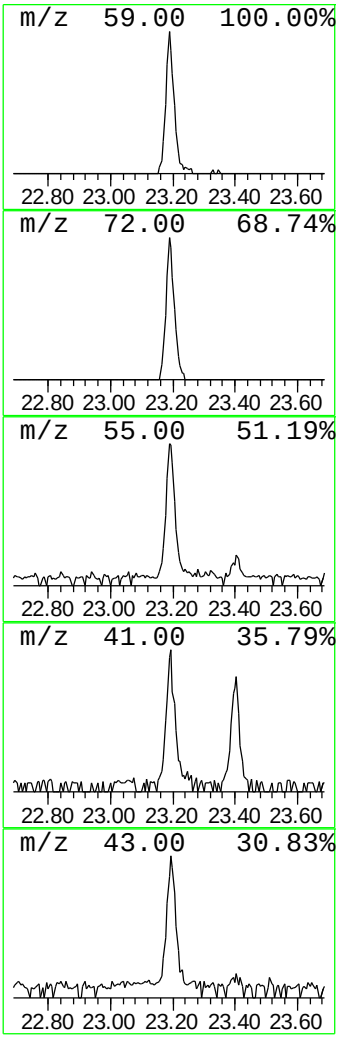
****

Peak Number 4 Hexadecanamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	7.24 ng/ul	74800	Chrysene-d12	21.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	53
2	d-Glucosamine	179	C6H13NO5	000090-77-7	50
3	Tetradecanamide	227	C14H29NO	000638-58-4	45
4	Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	38
5	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

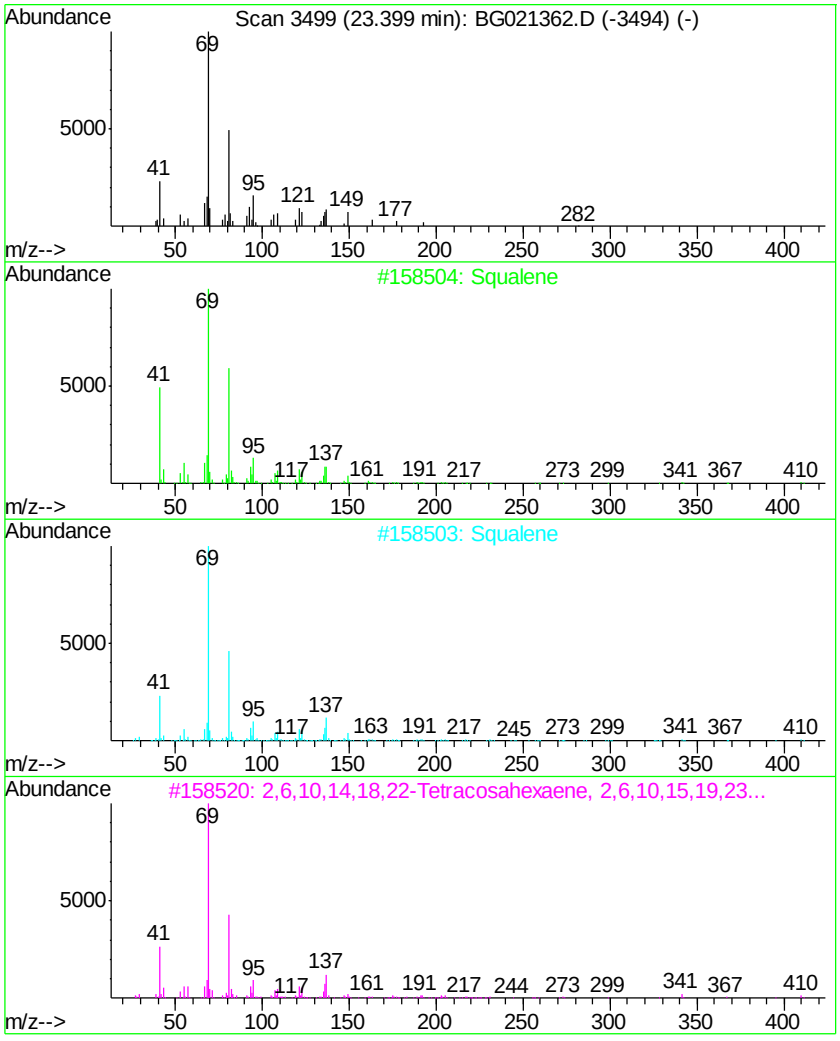
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

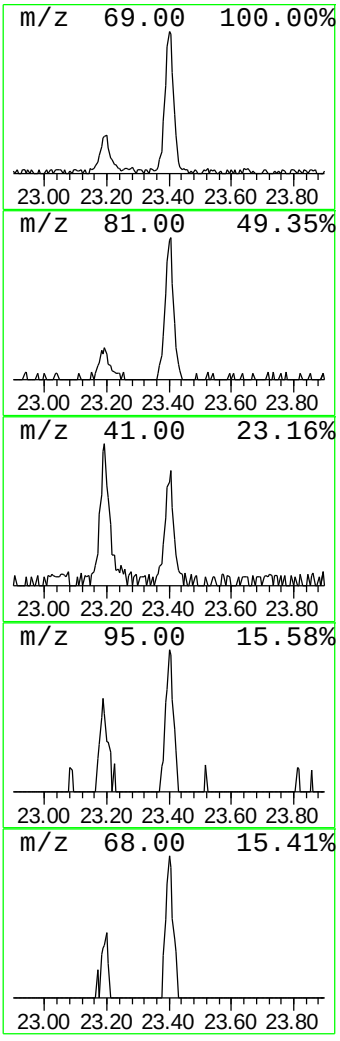
****

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	4.65 ng/ul	48026	Perylene-d12	24.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	007683-64-9	90
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	74
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG030816\
Data File : BG021362.D
Acq On : 8 Mar 2016 11:55
Operator : UM/SJ
Sample : H1655-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-DS-C70

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Str...	16.41	2.0	ng/ul	17814	4	17.47	175545	20.0
n-Hexadecanoic acid	18.33	2.5	ng/ul	21796	4	17.47	175545	20.0
(DEL) Alkane: Cyc...	21.35	13.6	ng/ul	140165	5	21.73	206657	20.0
Hexadecanamide	23.19	7.2	ng/ul	74800	5	21.73	206657	20.0
Squalene	23.40	4.7	ng/ul	48026	6	24.98	206555	20.0