LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BG060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.692	336	341	349	rVB	20347	34074	1.91%	0.293%
2	6.132	409	416	425	rVB	55769	102965	5.78%	0.885%
3	7.678	673	679	690	rVB2	44879	106435	5.97%	0.915%
4	8.077	740	747	755	rBV	116200	211474	11.87%	1.818%
5	8.541	819	826	836	rBV	225015	415658	23.33%	3.573%
6	8.870	872	882	891	rVB	195653	362892	20.36%	3.119%
7	9.699	1014	1023	1030	rBV	189212	374509	21.02%	3.219%
8	9.752	1030	1032	1039	rVB4	11661	18128	1.02%	0.156%
9	11.356	1298	1305	1313	rBV	329444	630896	35.40%	5.423%
10	13.741	1700	1711	1719	rBV	696189	1129630	63.39%	9.710%
11	14.440	1824	1830	1834	rBV2	24324	36772	2.06%	0.316%
12	14.552	1843	1849	1855	rBV	356176	549656	30.85%	4.725%
13	14.963	1912	1919	1925	rBV3	37577	64928	3.64%	0.558%
14	15.122	1937	1946	1953	rBV2	512705	873203	49.00%	7.506%
15	15.921	2077	2082	2089	rVB2	57539	84806	4.76%	0.729%
16	16.074	2104	2108	2114	rVB7	14242	24159	1.36%	0.208%
17	16.603	2191	2198	2206	rBV	282630	453810	25.47%	3.901%
18	16.861	2239	2242	2247	rVB3	16135	21657	1.22%	0.186%
19	16.943	2247	2256	2260	rBV3	36548	60887	3.42%	0.523%
20	17.572	2358	2363	2370	rBV	32689	49726	2.79%	0.427%
21	17.866	2406	2413	2426	rBV	587405	990502	55.58%	8.514%
22	18.318	2485	2490	2495	rBV3	11662	20786	1.17%	0.179%
23	18.600	2532	2538	2545	rBV	88016	213785	12.00%	1.838%
24	18.712	2551	2557	2566	rBV	284227	444112	24.92%	3.817%
25	19.828	2742	2747	2749	rBV4	16322	26823	1.51%	0.231%
26	19.963	2766	2770	2778	rBV2	101649	172141	9.66%	1.480%
27	20.222	2811	2814	2818	rBV4	16022	20875	1.17%	0.179%
28	20.445	2846	2852	2859	rVB	1309482	1781976	100.00%	15.317%
29	21.362	3003	3008	3015	rVB5	11363	28595	1.60%	0.246%
30	22.249	3151	3159	3168	rVB	570333	1104257	61.97%	9.492%
31	23.541	3374	3379	3384	rVB5	21089	38131	2.14%	0.328%
32	24.117	3470	3477	3483	rBV2	58055	127900	7.18%	1.099%
33	25.915	3772	3783	3798	rVB2	312605	1057694	59.36%	9.092%

LSC Area Percent Report

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Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BG060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 11633842

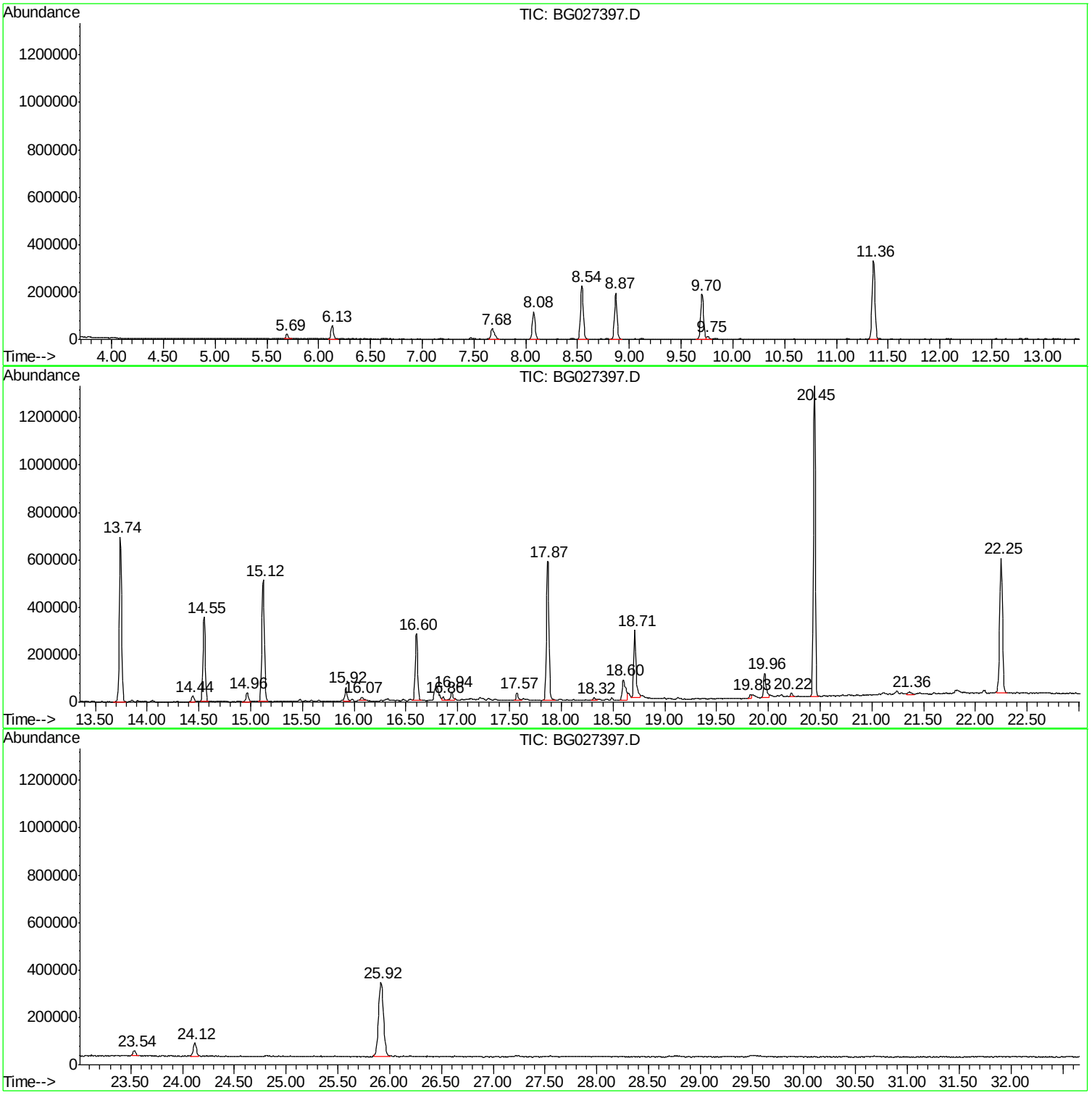
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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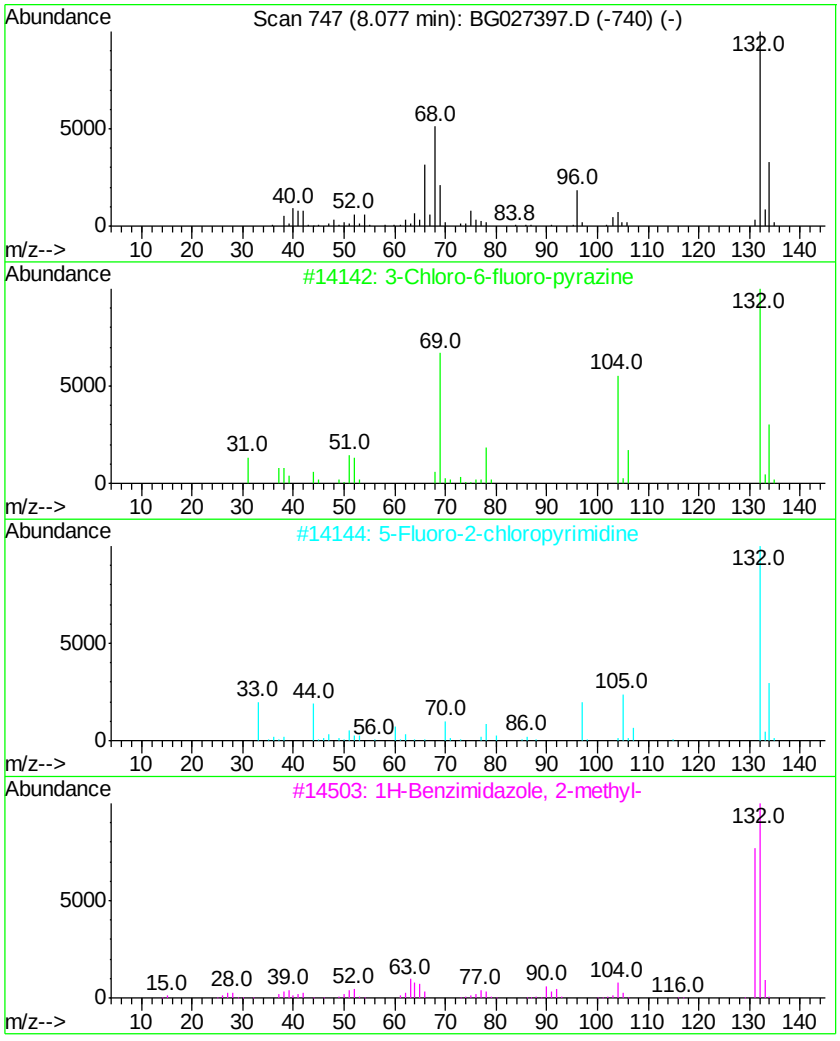
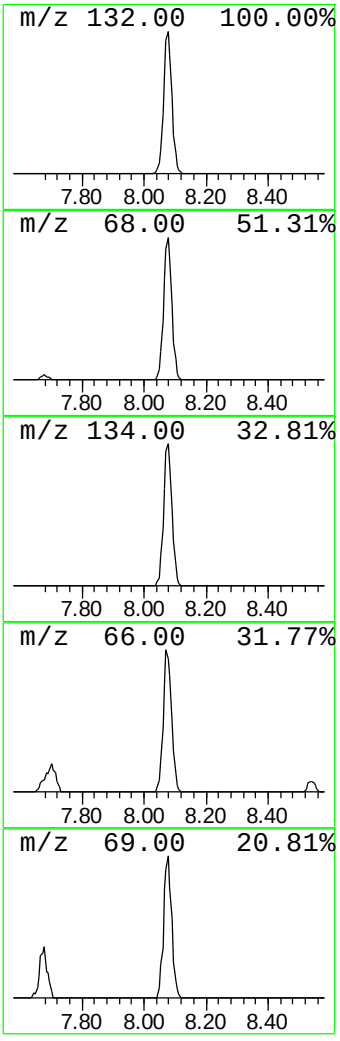
Peak Number 1 unknown8.08 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.08	10.18 ng	211474	1,4-Dichlorobenzene-d4	8.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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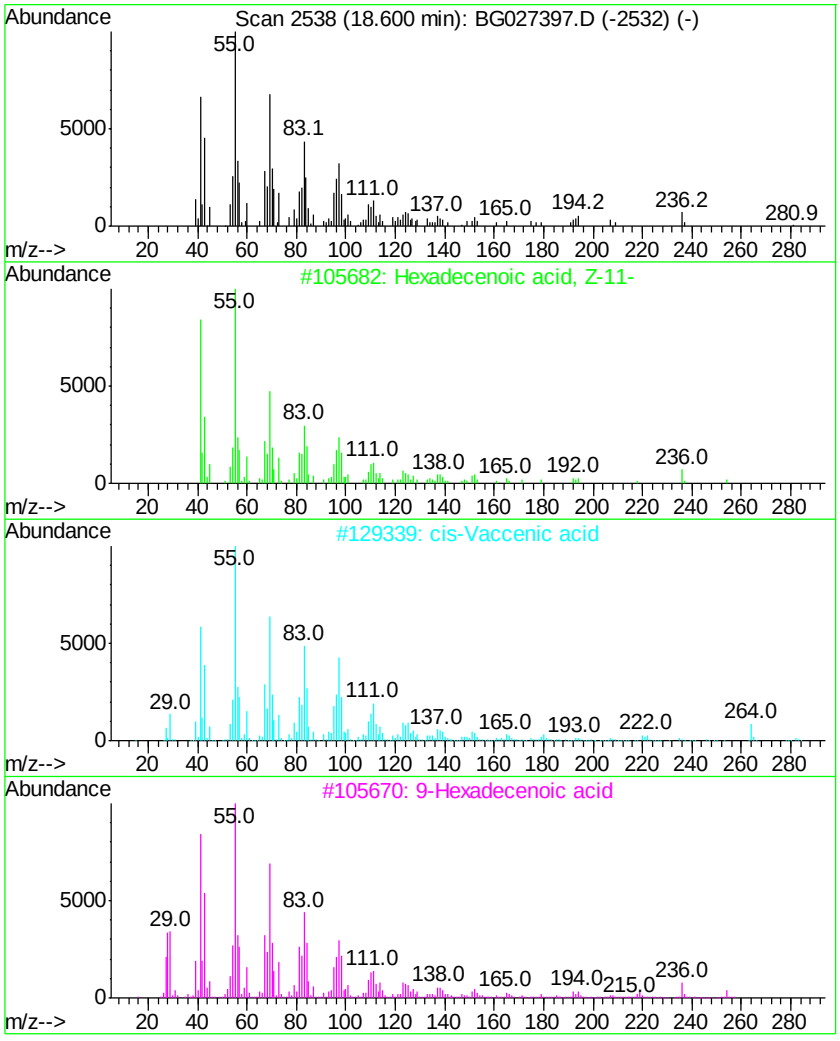
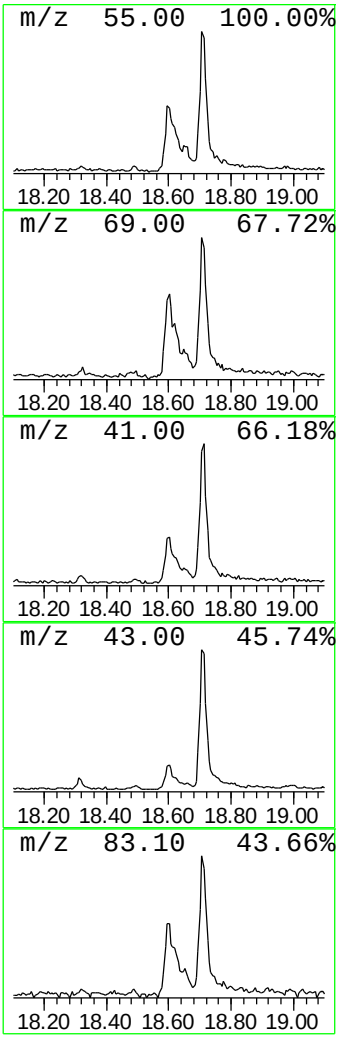
Peak Number 3 Hexadecenoic acid, Z-11- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.60	4.32 ng	213785	Phenanthrene-d10	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	90
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
3	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	87
4	Palmitoleic acid	254	C16H30O2	000373-49-9	83
5	9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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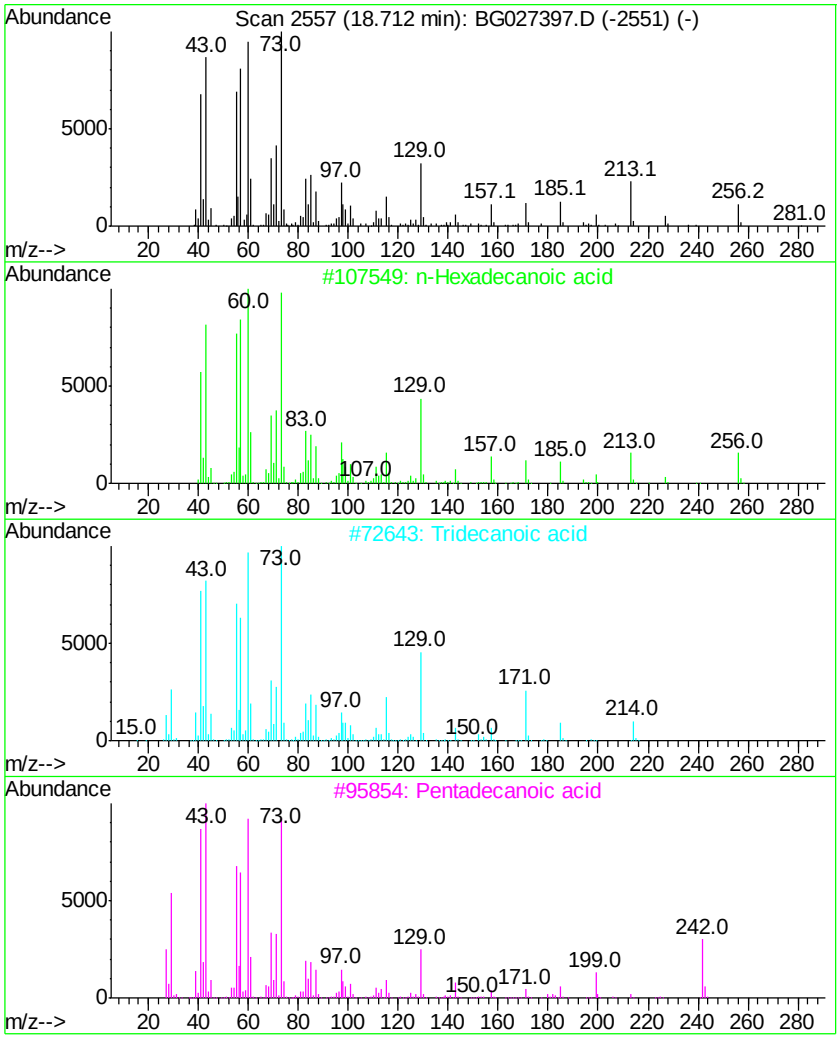
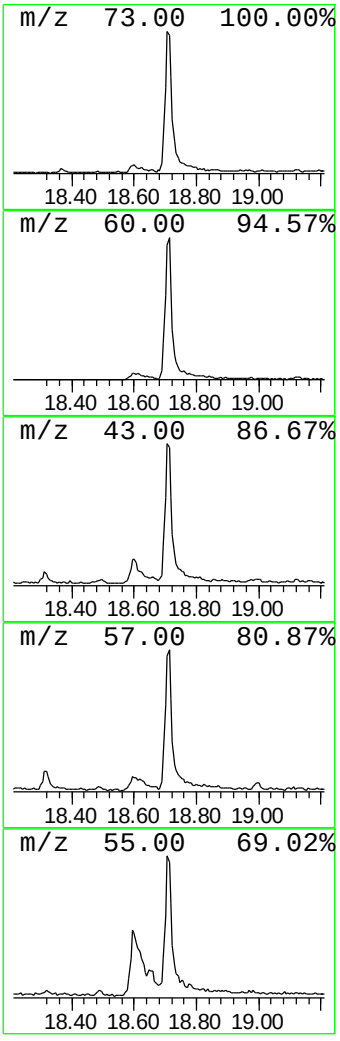
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.71	8.97 ng	444112	Phenanthrene-d10	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG061317\
Data File : BG027397.D
Acq On : 13 Jun 2017 22:19
Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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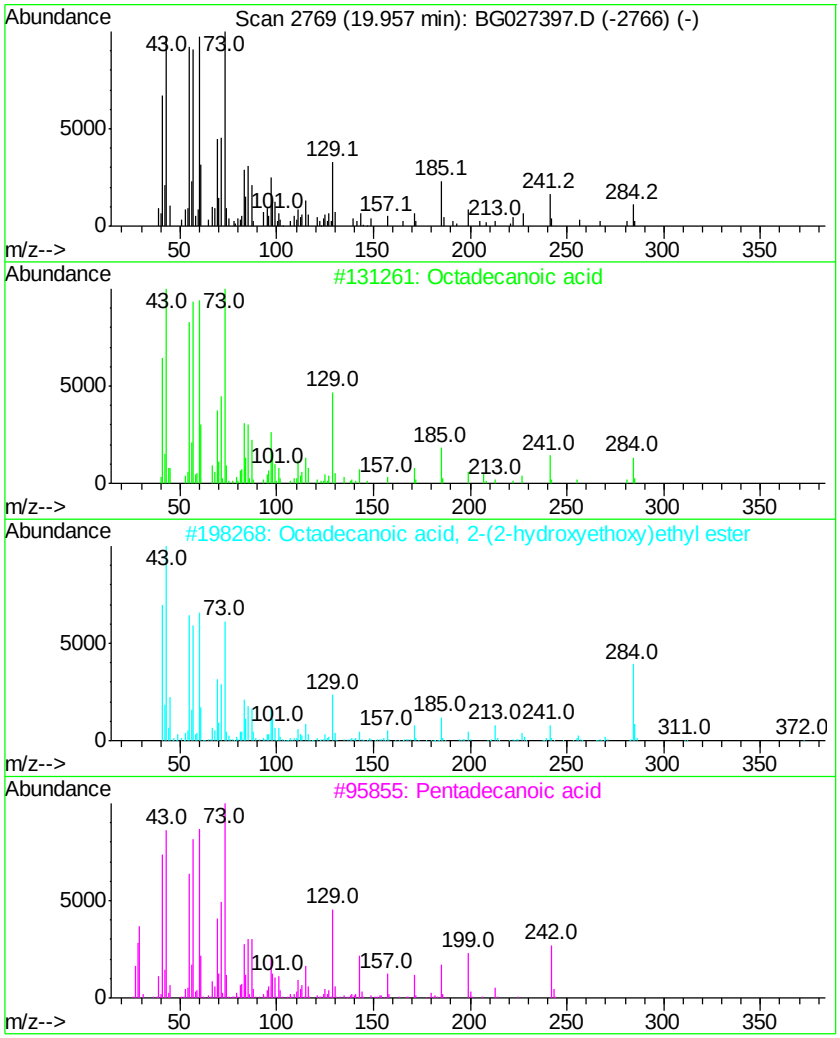
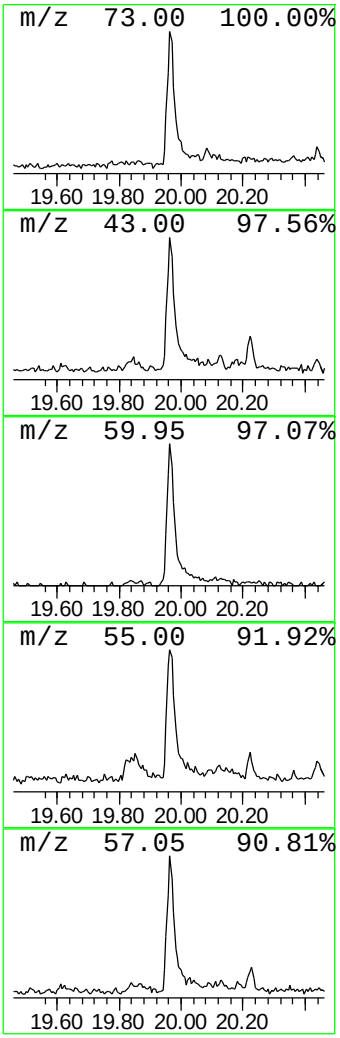
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.96	3.48 ng	172141	Phenanthrene-d10	17.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





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Operator : SJ/MA
Sample : I3614-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

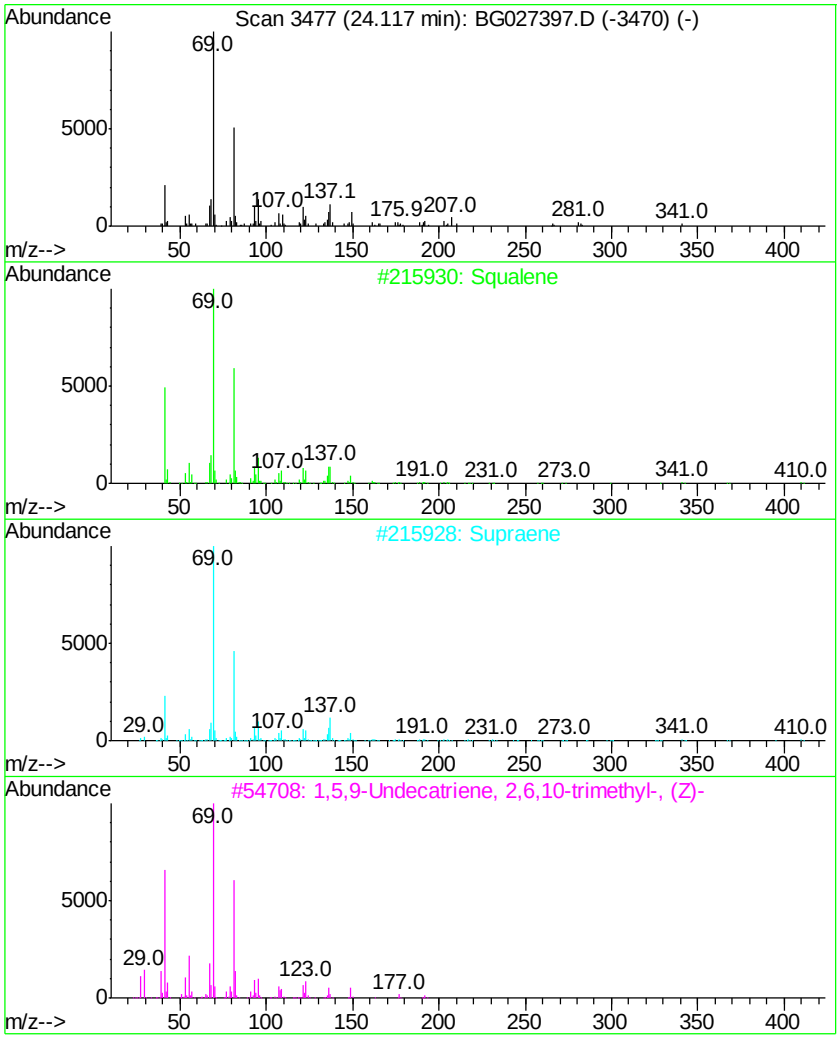
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

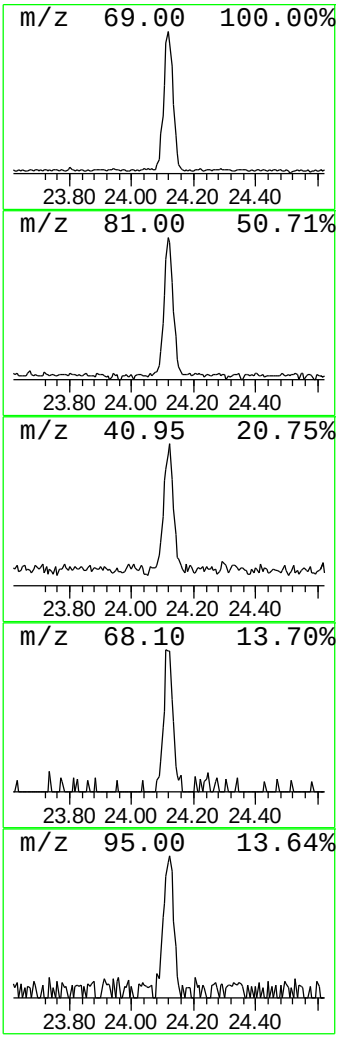
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	2.42 ng	127900	Perylene-d12	25.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	87
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
4	trans-Farnesol	222	C15H26O	000106-28-5	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061317\
Data File : BG027397.D
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Sample : I3614-07
Misc :
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Instrument : BNA_G
ClientSampleId : PZ-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown8.08	8.08	10.2	ng	211474	1	8.54	415658	20.0
Hexadecenoic acid...	18.60	4.3	ng	213785	4	17.87	990502	20.0
n-Hexadecanoic acid	18.71	9.0	ng	444112	4	17.87	990502	20.0
Octadecanoic acid	19.96	3.5	ng	172141	4	17.87	990502	20.0
Squalene	24.12	2.4	ng	127900	6	25.92	1057690	20.0