LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF033117\
Data File : BF094094.D
Acq On : 31 Mar 2017 14:21
Operator : SJ/MA
Sample : I2474-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49B-9-11

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_F\METHODS\8270-BF032217.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	4.046	362	367	376	rVB	359373	467044	10.73%	1.247%
2	4.440	429	434	437	rBV	3579009	3525395	80.98%	9.409%
3	5.504	608	615	620	rBV	3198600	3779493	86.82%	10.087%
4	5.645	633	639	642	rBV	3528687	3823157	87.82%	10.204%
5	5.898	677	682	685	rBV	1027226	991947	22.79%	2.647%
6	6.075	707	712	716	rBV	3001356	3038414	69.79%	8.109%
7	6.545	785	792	795	rBV	2133240	2461396	56.54%	6.569%
8	7.398	931	937	941	rBV	1280334	1341500	30.82%	3.580%
9	8.722	1155	1162	1166	rBV	3619852	4353346	100.00%	11.619%
10	8.904	1188	1193	1199	rVB	64768	67906	1.56%	0.181%
11	9.216	1240	1246	1250	rBV	508436	530133	12.18%	1.415%
12	9.539	1291	1301	1309	rBV2	1390045	1487754	34.17%	3.971%
13	10.133	1397	1402	1406	rVB	57226	56317	1.29%	0.150%
14	10.516	1460	1467	1470	rBV	1946619	2246892	51.61%	5.997%
15	10.716	1496	1501	1504	rBV	58234	71243	1.64%	0.190%
16	11.363	1605	1611	1615	rBV	1382389	1410368	32.40%	3.764%
17	11.710	1666	1670	1681	rBV	187048	239220	5.50%	0.638%
18	12.721	1838	1842	1851	rBV	644378	748584	17.20%	1.998%
19	13.174	1913	1919	1923	rBV2	36085	53129	1.22%	0.142%
20	13.345	1939	1948	1952	rBV2	3276077	3708802	85.19%	9.898%
21	13.933	2045	2048	2053	rBV	68731	89257	2.05%	0.238%
22	14.515	2140	2147	2159	rBV3	197795	345300	7.93%	0.922%
23	14.615	2159	2164	2168	rVV	1210008	1246582	28.64%	3.327%
24	14.668	2168	2173	2180	rVB	72640	101105	2.32%	0.270%
25	15.468	2305	2309	2314	rVB	253983	256050	5.88%	0.683%
26	15.727	2348	2353	2358	rBV	115814	129322	2.97%	0.345%
27	16.245	2436	2441	2449	rBV	785729	898697	20.64%	2.399%

Sum of corrected areas: 37468353

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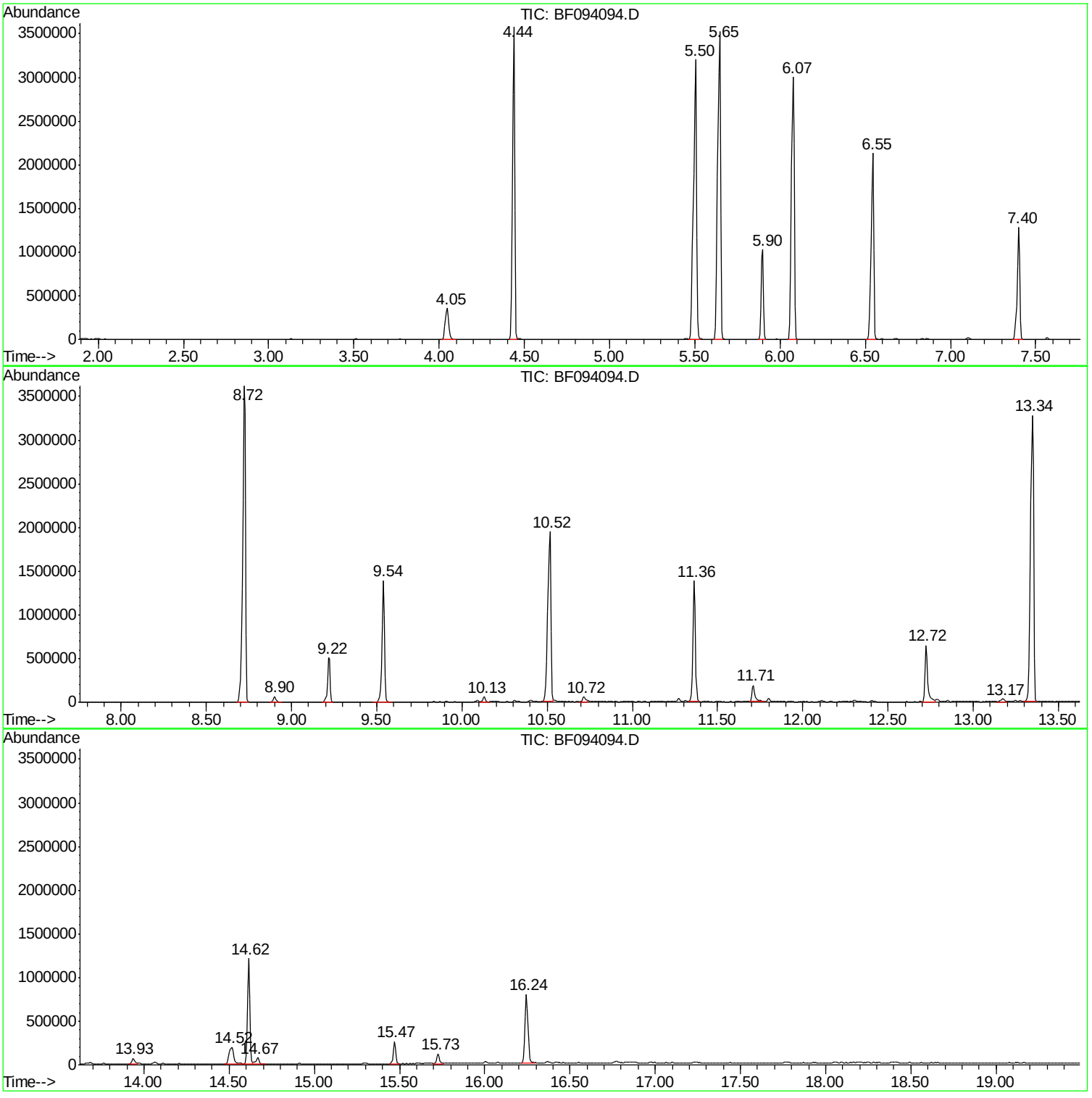
Instrument :
BNA_F
ClientSampleId :
49B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\Data\BF033117\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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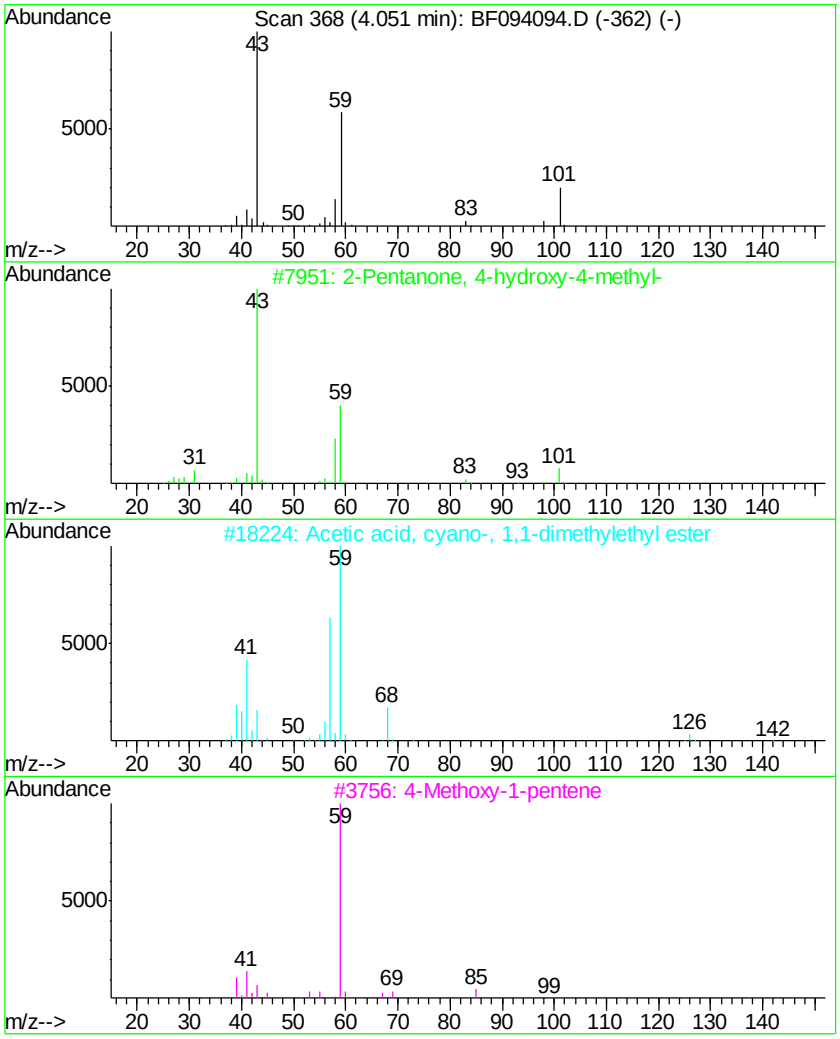
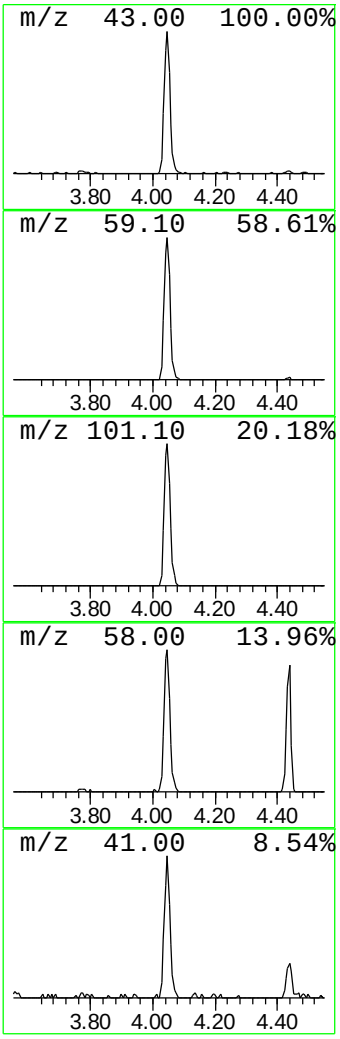
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.05	9.42 ng	467044	1,4-Dichlorobenzene-d4	5.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Sample : I2474-01
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Instrument : BNA_F
ClientSampleId : 49B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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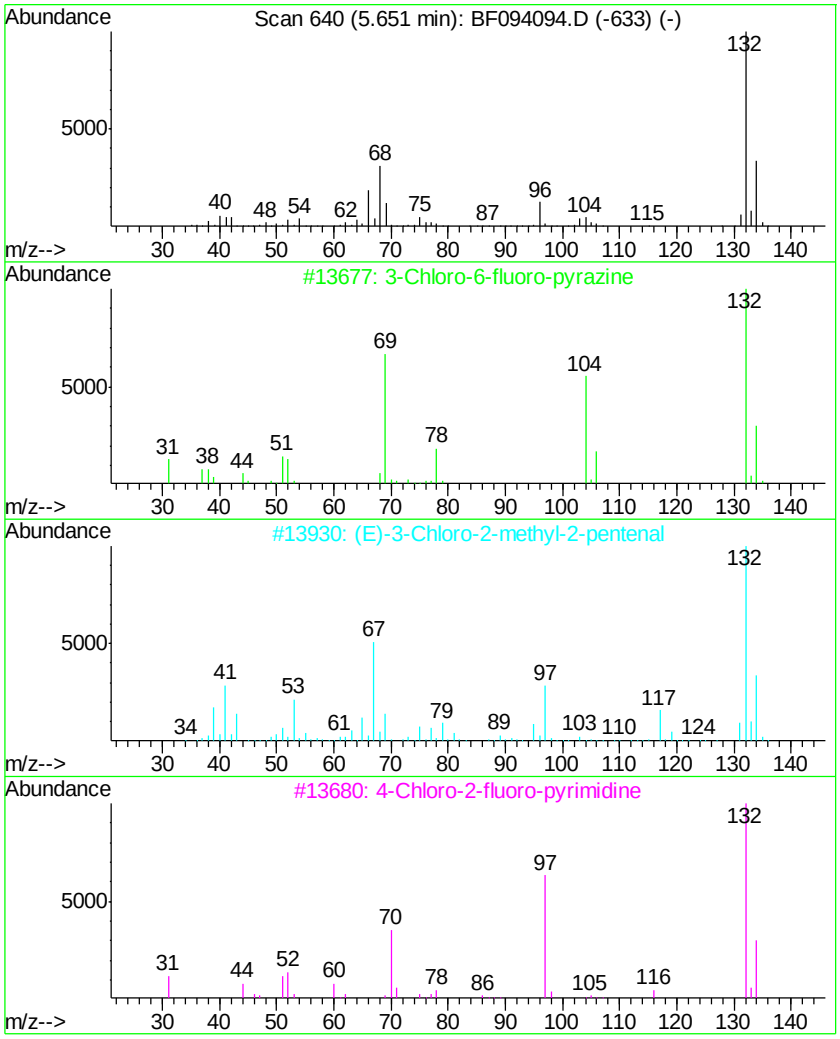
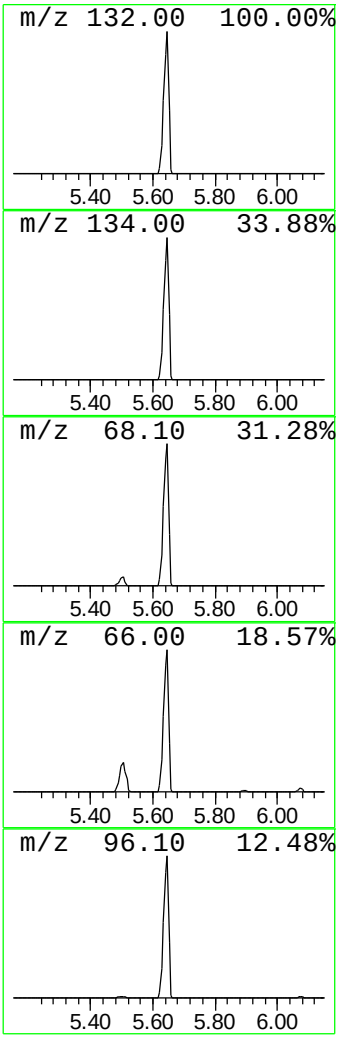
Peak Number 2 unknown5.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	77.08 ng	3823160	1,4-Dichlorobenzene-d4	5.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF094094.D
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Operator : SJ/MA
Sample : I2474-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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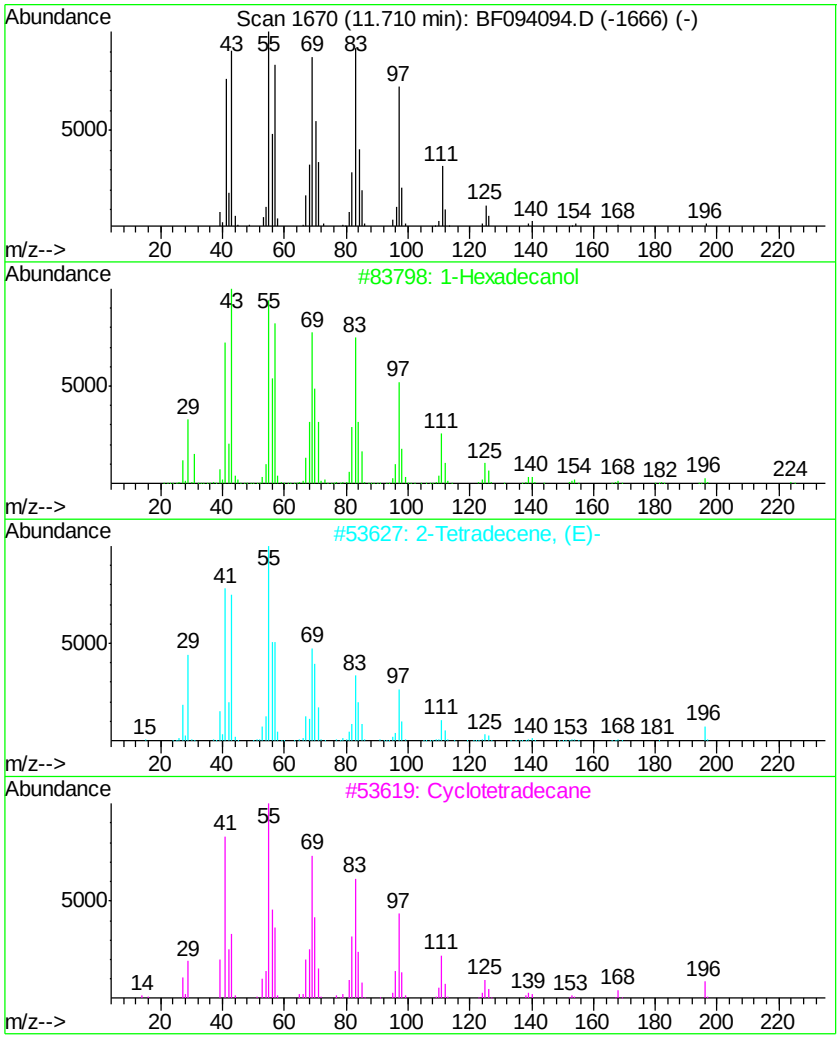
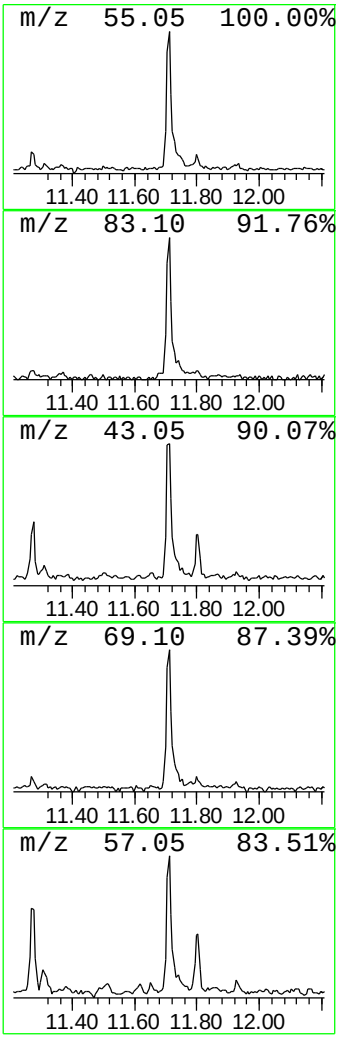
Peak Number 4 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	3.39 ng	239220	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	2-Tetradecene, (E)-	196	C14H28	035953-53-8	94
3	Cyclotetradecane	196	C14H28	000295-17-0	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	1-Tetradecene	196	C14H28	001120-36-1	91





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Operator : SJ/MA
Sample : I2474-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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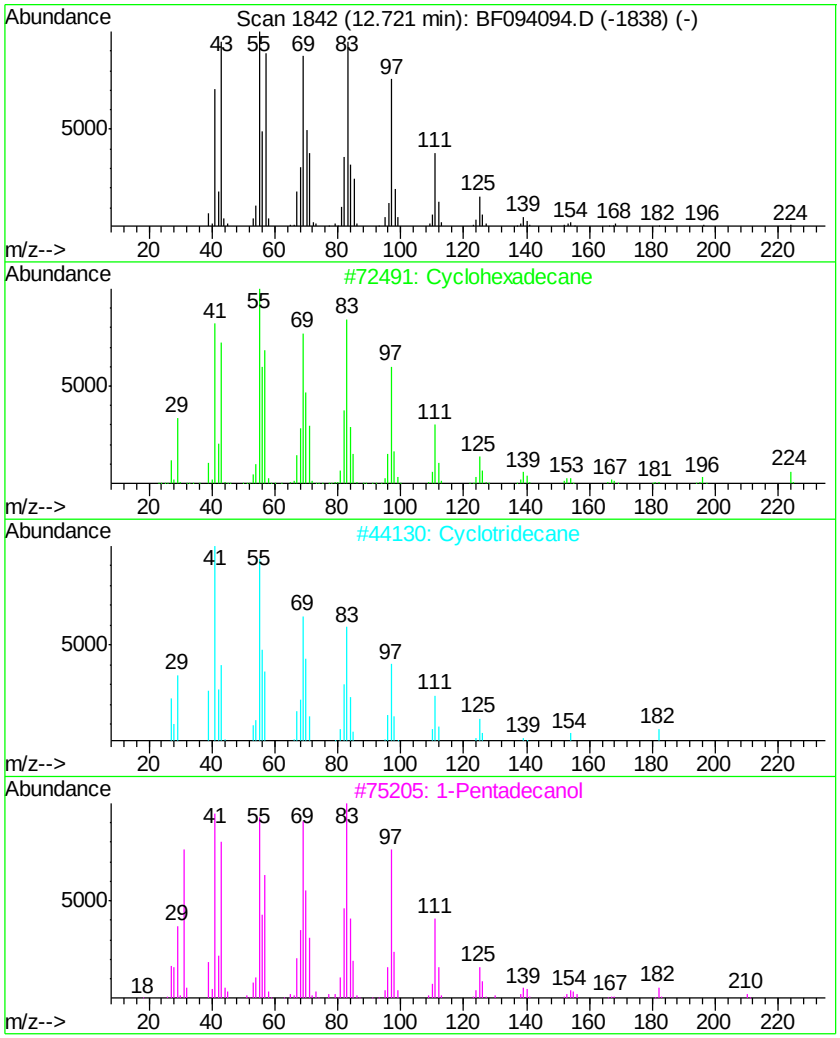
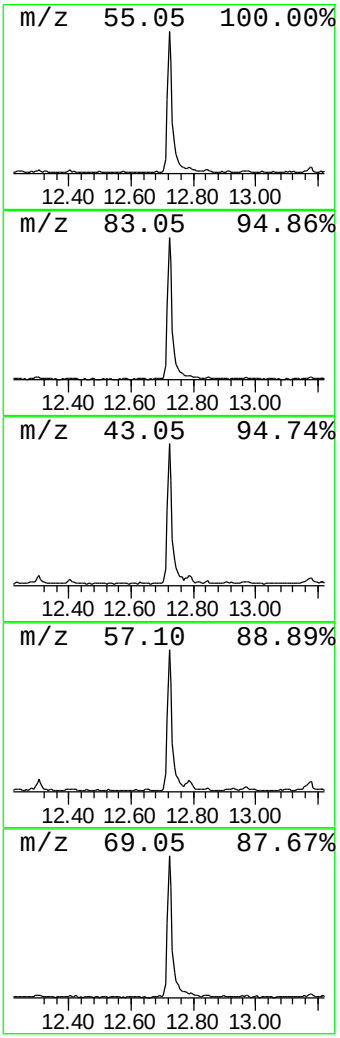
Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	10.62 ng	748584	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Cyclotridecane	182	C13H26	000295-02-3	93
3	1-Pentadecanol	228	C15H32O	000629-76-5	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91





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Sample : I2474-01
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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49B-9-11

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TIC Integration Parameters: LSCINT.P

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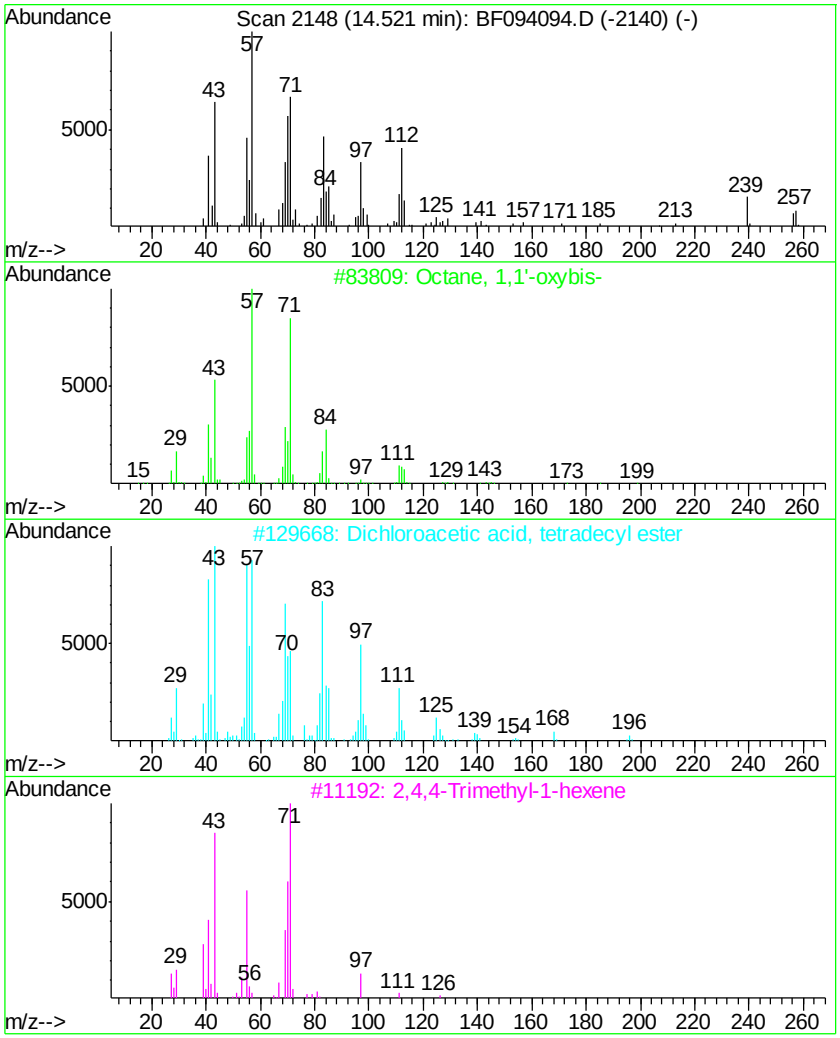
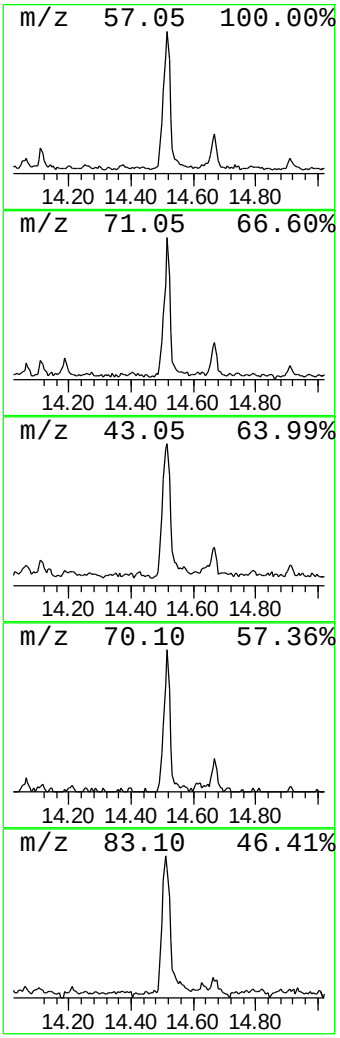
Peak Number 6 unknown14.52 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	5.54 ng	345300	Chrysene-d12	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	43
2	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	41
3	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	38
4	Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	38
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	38





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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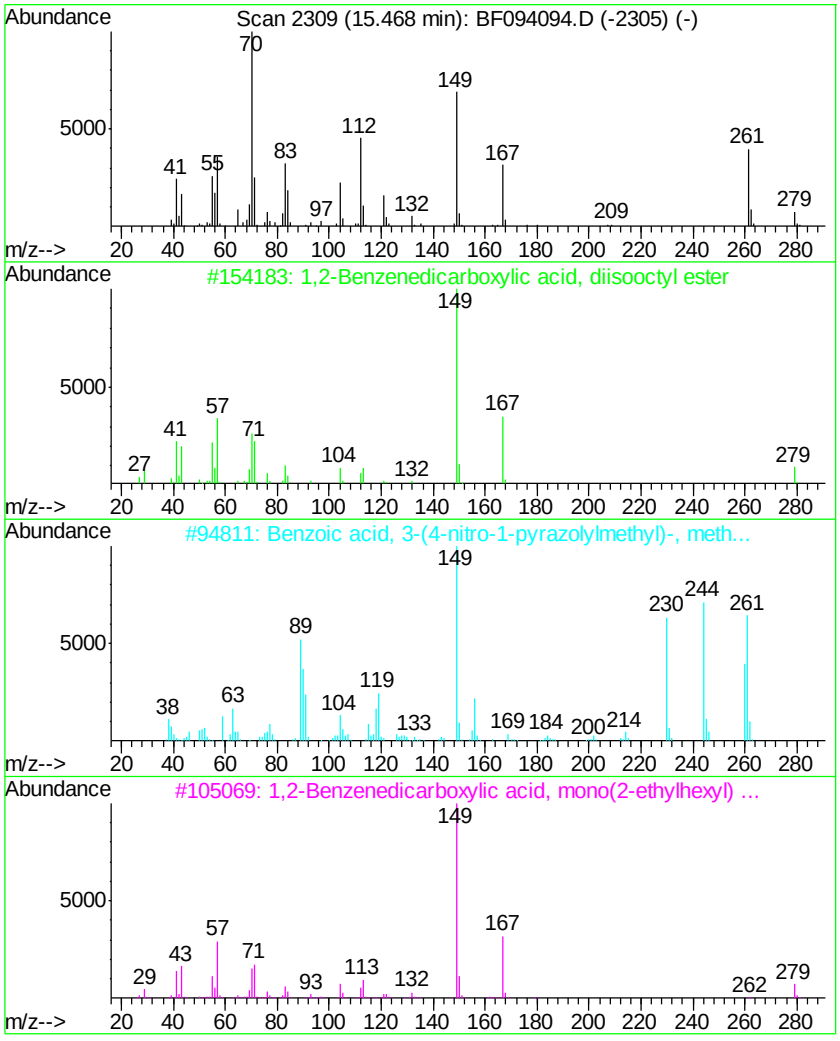
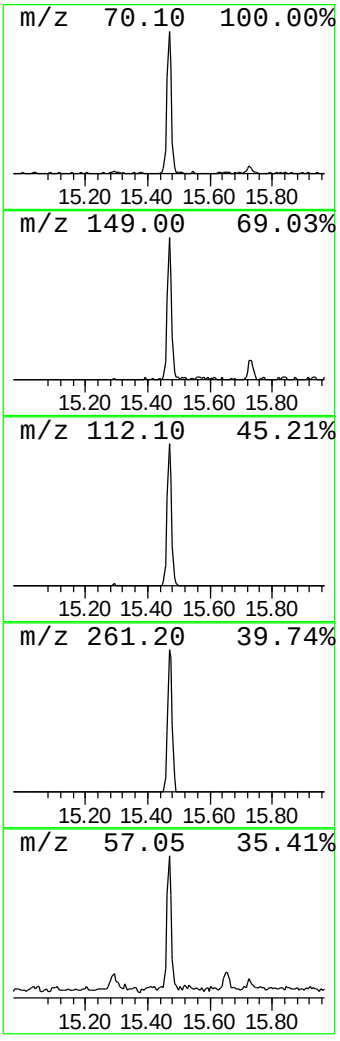
Peak Number 7 unknown15.47 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	5.70 ng	256050	Perylene-d12	16.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	22
2	Benzoic acid, 3-(4-nitro-1-pyraz...	261	C12H11N3O4	1000273-84-4	22
3	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	22
4	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	17
5	5-Undecene, 3-methyl-, (E)-	168	C12H24	074630-67-4	14





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

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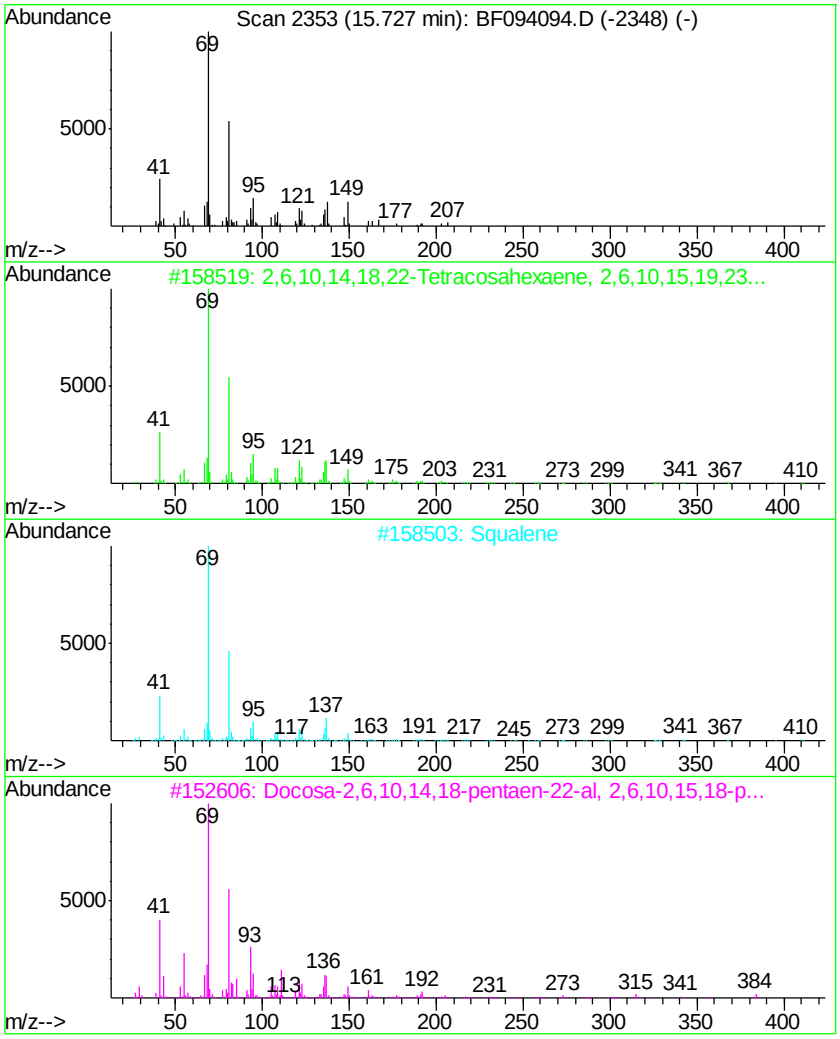
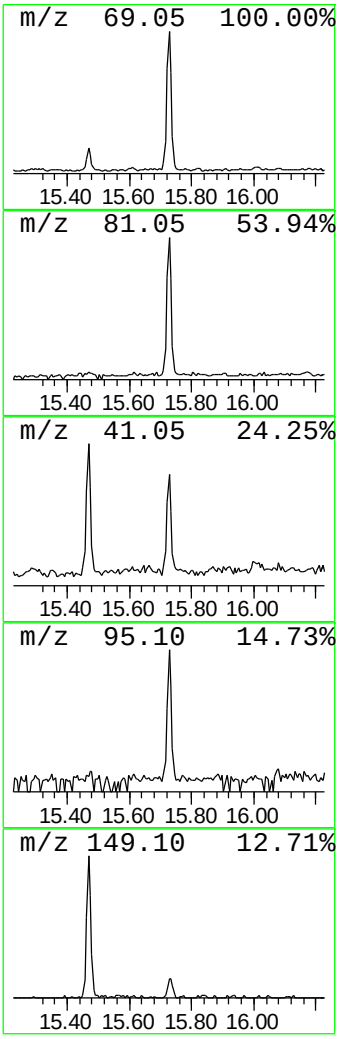
Peak Number 8 2,6,10,14,18,22-Tetracosahe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.88 ng	129322	Perylene-d12	16.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
2	Squalene	410	C30H50	007683-64-9	87
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	68
5	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.05	9.4	ng	467044	1	5.90	991947	20.0
unknown5.65	5.65	77.1	ng	3823160	1	5.90	991947	20.0
1-Hexadecanol	11.71	3.4	ng	239220	4	11.36	1410370	20.0
Cyclohexadecane	12.72	10.6	ng	748584	4	11.36	1410370	20.0
unknown14.52	14.52	5.5	ng	345300	5	14.62	1246580	20.0
unknown15.47	15.47	5.7	ng	256050	6	16.24	898697	20.0
2,6,10,14,18,22-T...	15.73	2.9	ng	129322	6	16.24	898697	20.0