LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040618\
Data File : BF104354.D
Acq On : 7 Apr 2018 12:55
Operator : JU/SJ
Sample : J2255-09
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 040418-DBRI-E-D-S

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-BF040618.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	4.998	491	495	500	rVB	153106	153970	4.18%	0.694%
2	5.404	559	564	567	rBV	1044379	987257	26.77%	4.449%
3	6.416	732	736	744	rVB	789700	625279	16.95%	2.818%
4	6.563	757	761	765	rBV	1971120	1891894	51.30%	8.527%
5	6.804	798	802	805	rBV	952264	824774	22.36%	3.717%
6	6.957	824	828	832	rVB	2700089	2573444	69.78%	11.598%
7	7.369	892	898	901	rBV	2142596	2062257	55.92%	9.294%
8	8.086	1016	1020	1023	rVB	1320415	1088923	29.53%	4.908%
9	9.163	1198	1203	1206	rBV	3872883	3687897	100.00%	16.621%
10	9.551	1266	1269	1273	rBV	107079	103016	2.79%	0.464%
11	9.769	1303	1306	1309	rBV	98481	77488	2.10%	0.349%
12	9.839	1314	1318	1322	rVB2	1350157	1161624	31.50%	5.235%
13	10.269	1384	1391	1394	rBV2	107224	102812	2.79%	0.463%
14	10.627	1447	1452	1455	rBV	1564359	1325328	35.94%	5.973%
15	10.745	1469	1472	1480	rVB	101499	93902	2.55%	0.423%
16	11.327	1567	1571	1574	rBV	1131393	913643	24.77%	4.118%
17	11.851	1657	1660	1670	rBV2	45918	45358	1.23%	0.204%
18	12.739	1808	1811	1817	rVB	142172	108885	2.95%	0.491%
19	12.915	1837	1841	1845	rBV	2539582	2503803	67.89%	11.284%
20	13.445	1928	1931	1934	rBV	82913	66197	1.79%	0.298%
21	13.815	1990	1994	2000	rBV	80381	88283	2.39%	0.398%
22	13.968	2016	2020	2023	rBV	895982	767841	20.82%	3.461%
23	14.827	2163	2166	2171	rVB	102017	101127	2.74%	0.456%
24	15.427	2263	2268	2272	rBV	605492	691731	18.76%	3.118%
25	15.468	2272	2275	2282	rVB2	32377	42843	1.16%	0.193%
26	15.898	2342	2348	2353	rBV	30131	46365	1.26%	0.209%
27	16.398	2425	2433	2441	rBV2	25515	52444	1.42%	0.236%

Sum of corrected areas: 22188385

LSC Report - Integrated Chromatogram

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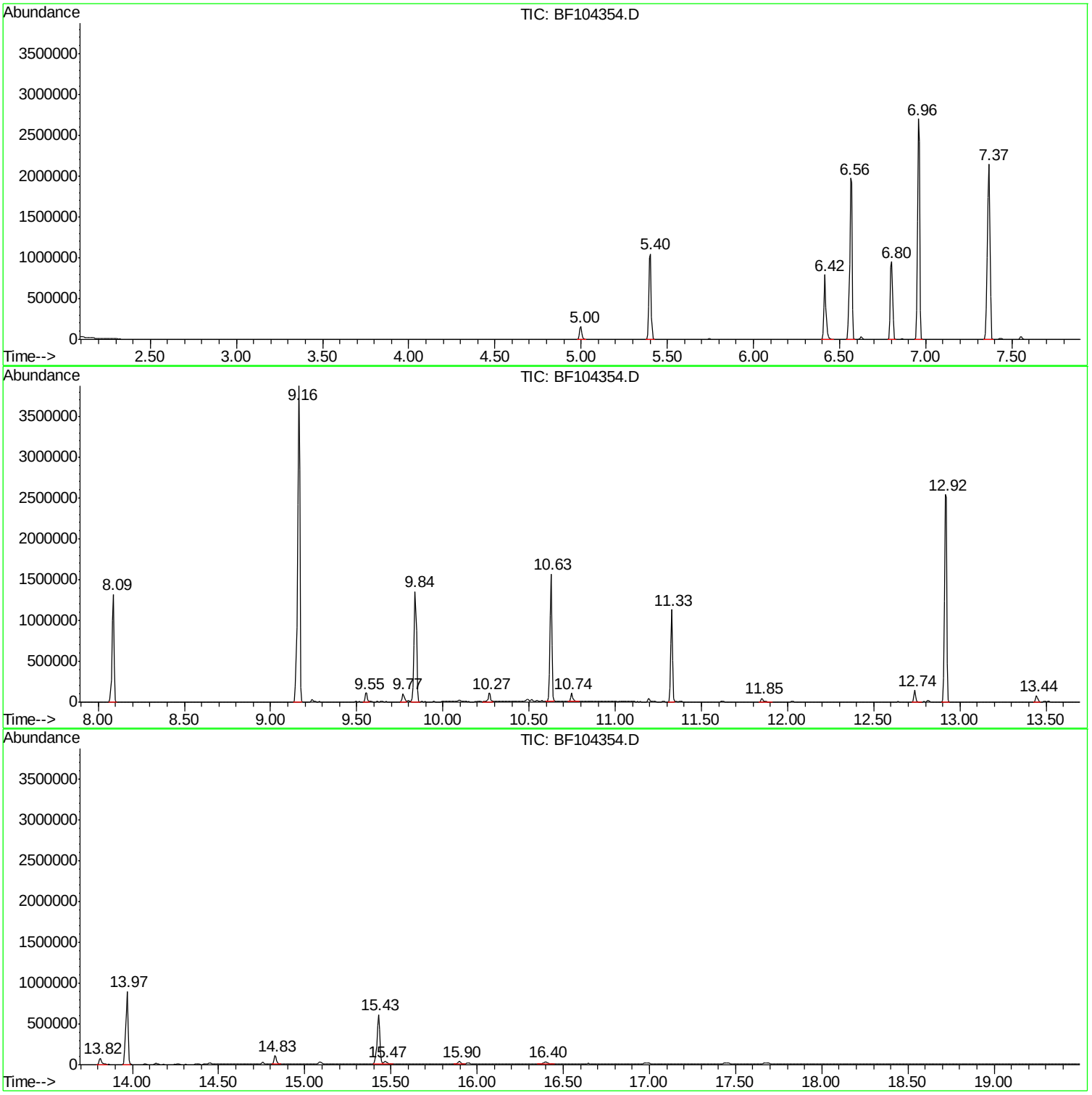
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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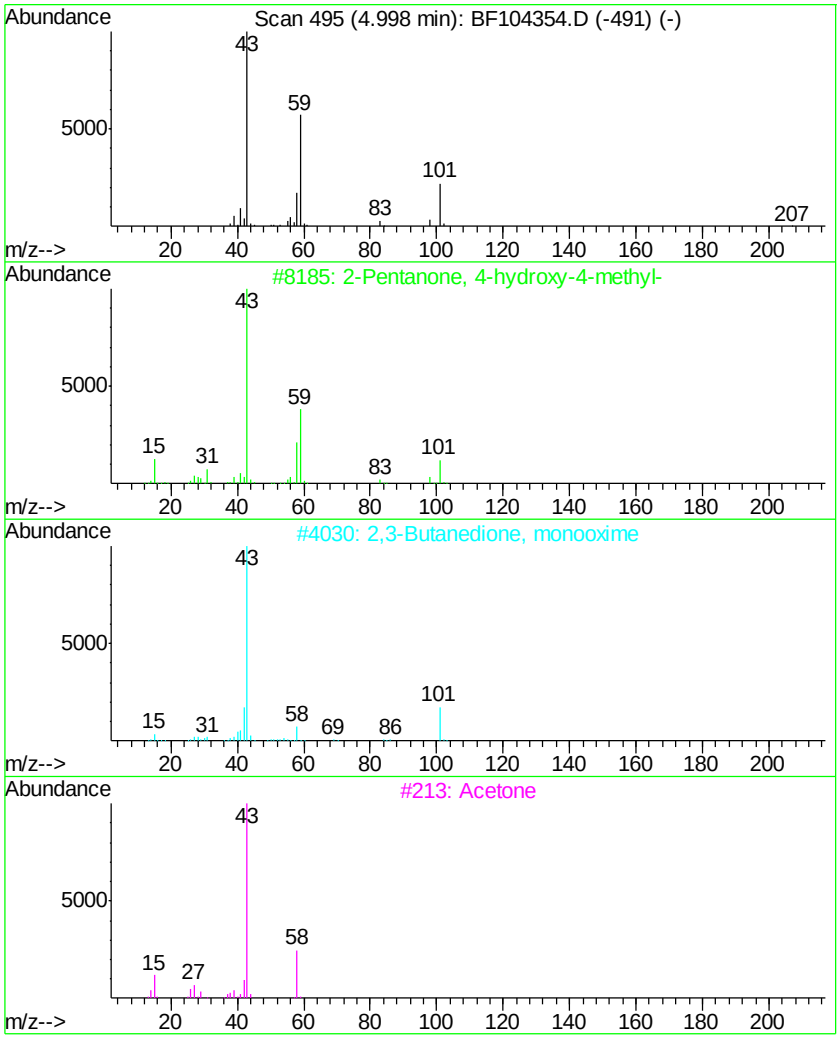
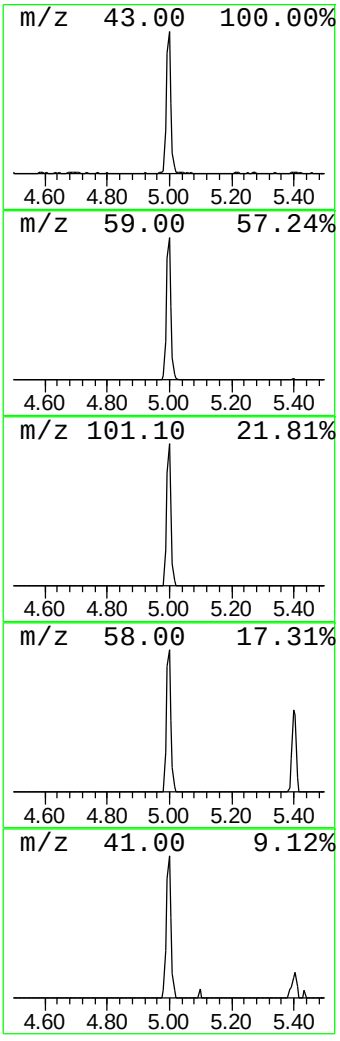
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.73 ng	153970	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Acetone	58	C3H6O	000067-64-1	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : 040418-DBRI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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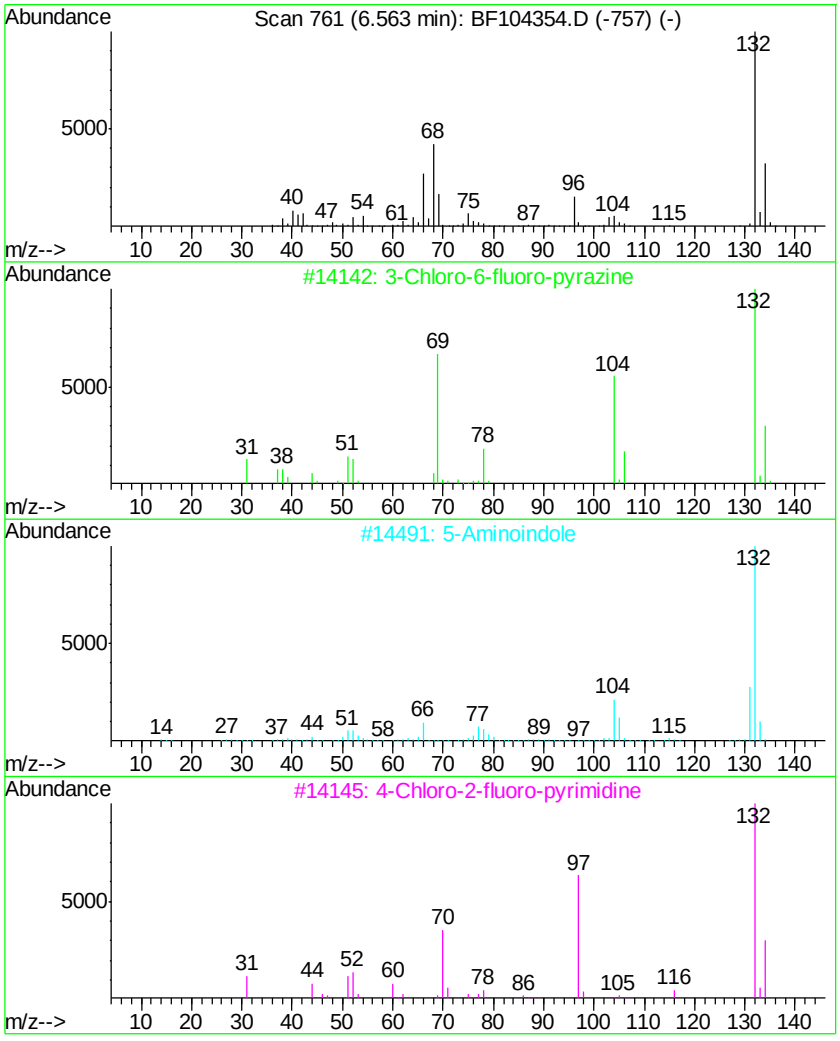
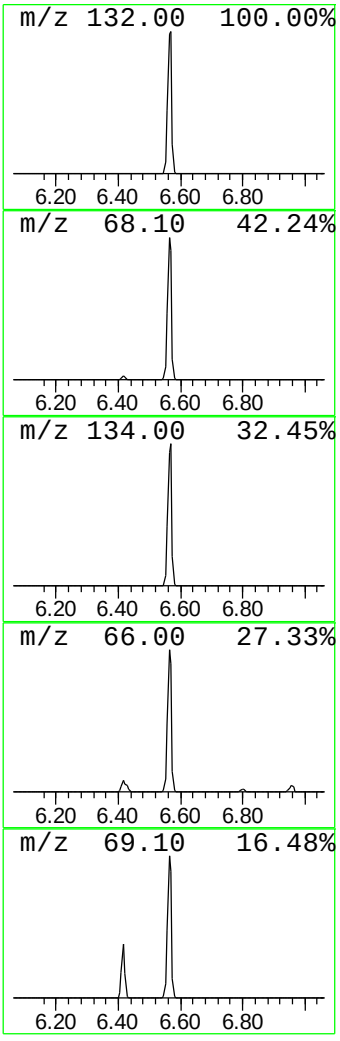
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	45.88 ng	1891890	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
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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Instrument : BNA_F
ClientSampleId : 040418-DBRI-E-D-S

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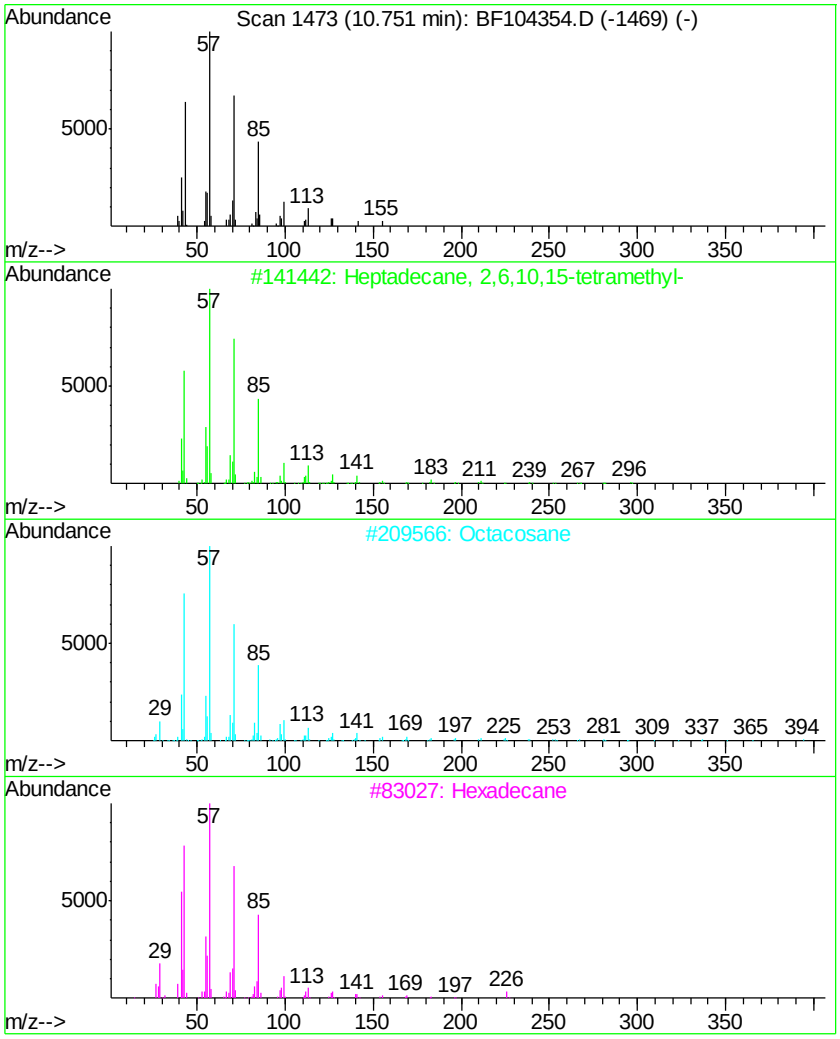
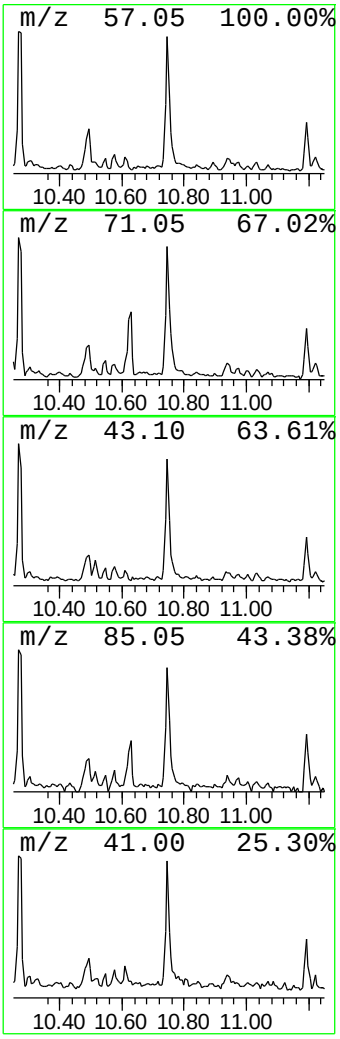
Peak Number 4 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.06 ng	93902	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Hexadecane	226	C16H34	000544-76-3	87
4	Heptacosane	380	C27H56	000593-49-7	86
5	Tetradecane	198	C14H30	000629-59-4	86





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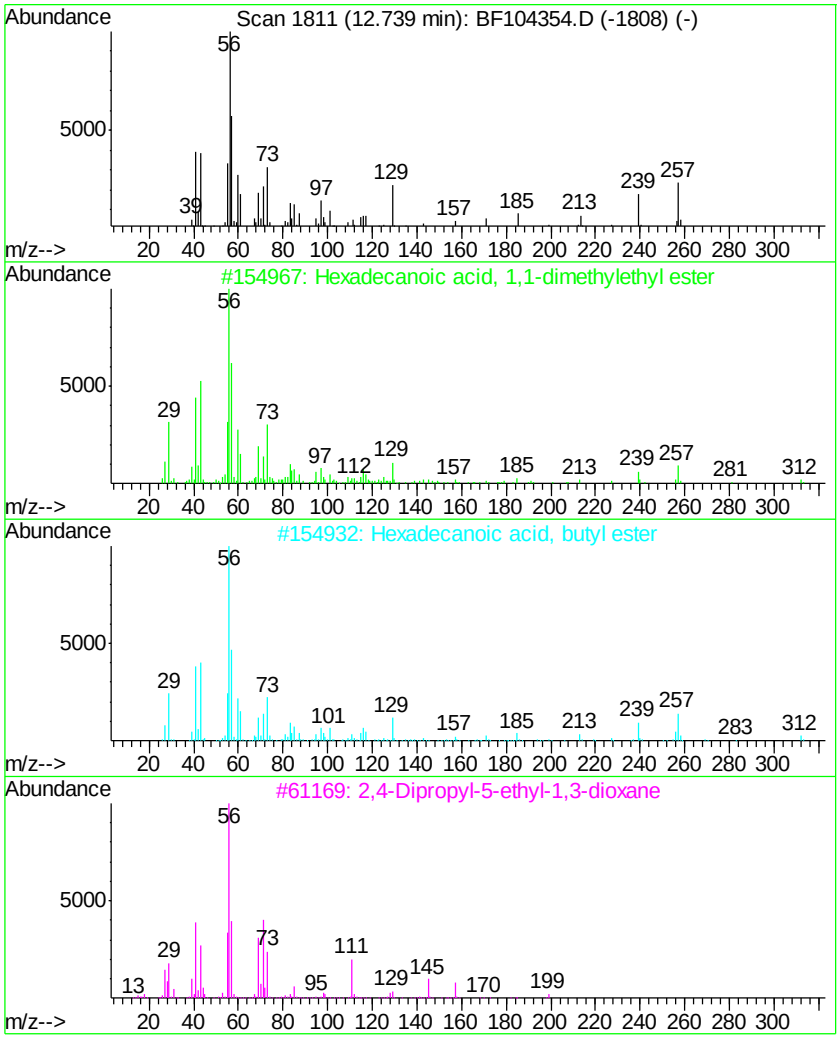
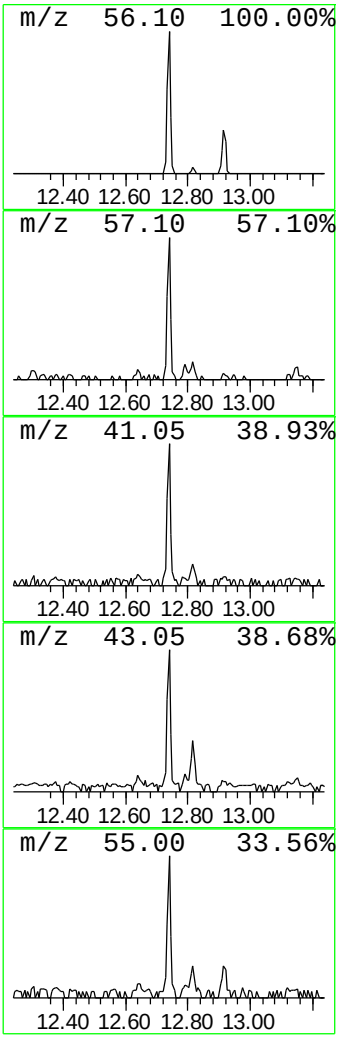
Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.84 ng	108885	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	49
3	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	27





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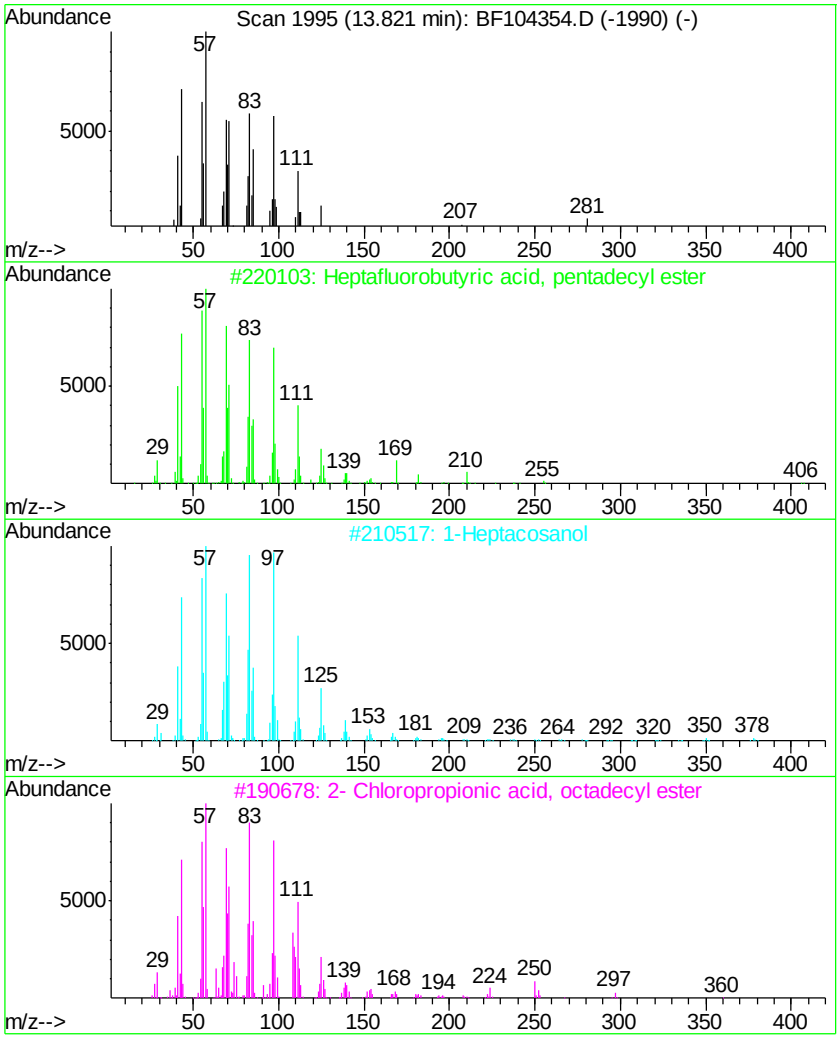
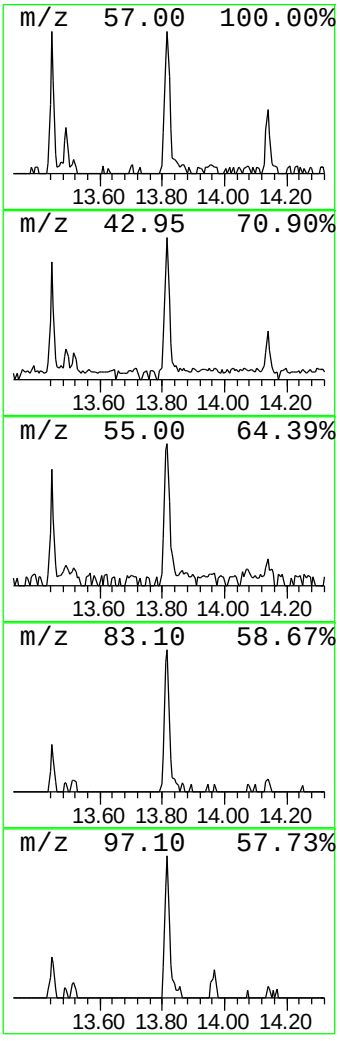
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.30 ng	88283	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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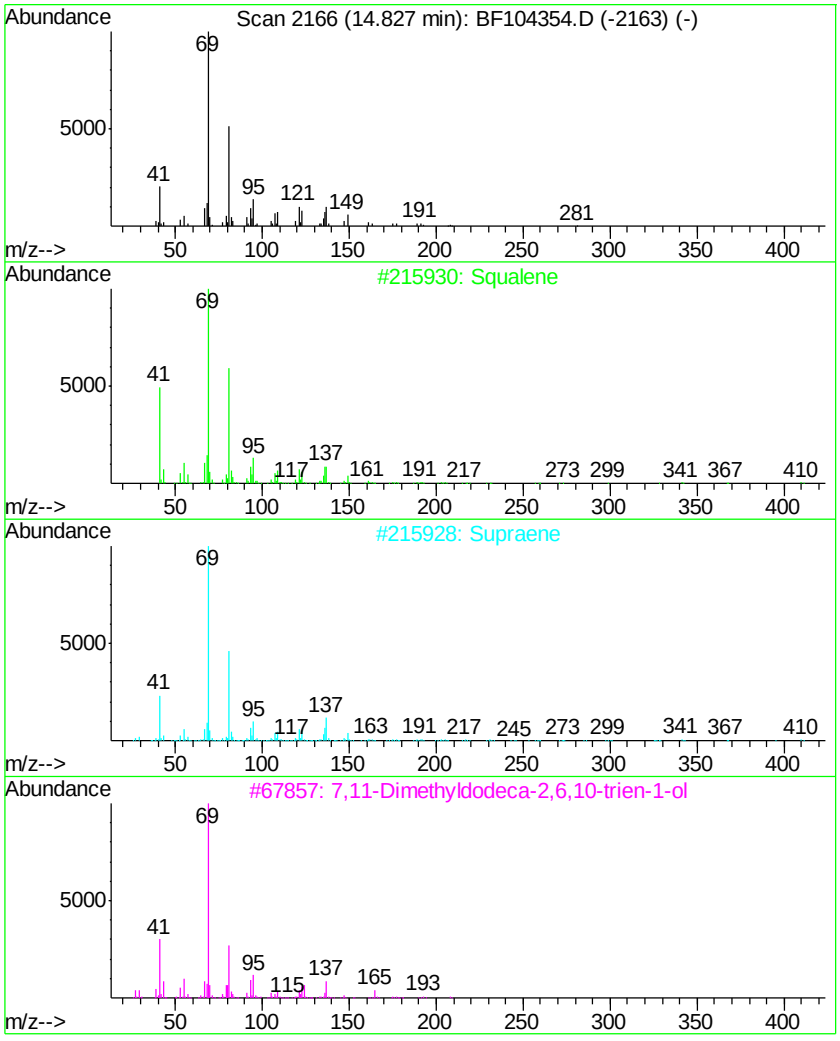
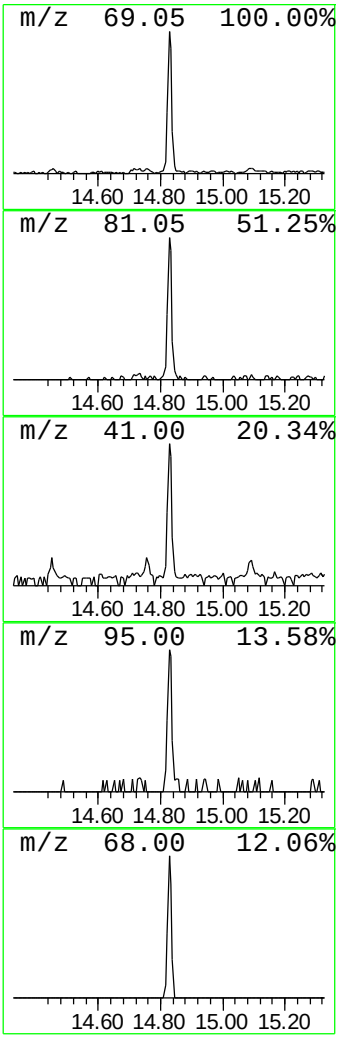
Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.92 ng	101127	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	59
5	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	53





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.7	ng	153970	1	6.80	824774	20.0
unknown6.56	6.56	45.9	ng	1891890	1	6.80	824774	20.0
Heptadecane, 2,6,...	10.75	2.1	ng	93902	4	11.33	913643	20.0
Hexadecanoic acid...	12.74	2.8	ng	108885	5	13.97	767841	20.0
Heptafluorobutyri...	13.82	2.3	ng	88283	5	13.97	767841	20.0
Squalene	14.83	2.9	ng	101127	6	15.43	691731	20.0