LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082515.D
Acq On : 24 Oct 2015 15:53
Operator : UM/IZ
Sample : G4117-17
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-03(0-2)

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-BF101015.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	4.926	240	244	255	rBV	803199	1367284	51.70%	6.278%
2	5.360	280	282	284	rBV	2147414	2171460	82.10%	9.970%
3	5.749	314	316	320	rVB	28796	27805	1.05%	0.128%
4	6.411	371	374	376	rBV	2069575	2276536	86.07%	10.452%
5	6.526	382	384	387	rBV	2294897	2126293	80.39%	9.762%
6	6.754	402	404	406	rBV	654577	559165	21.14%	2.567%
7	6.914	415	418	420	rBV	1590433	1812448	68.53%	8.321%
8	7.326	451	454	457	rBV	1132528	1190123	45.00%	5.464%
9	8.046	514	517	519	rBV	798870	736130	27.83%	3.380%
10	9.132	609	612	614	rBV	1903354	2644843	100.00%	12.143%
11	9.520	644	646	649	rBV	411437	381715	14.43%	1.753%
12	9.806	668	671	673	rBV	670342	790898	29.90%	3.631%
13	10.229	707	708	710	rVB	40437	30601	1.16%	0.140%
14	10.595	737	740	743	rBV	1288285	1218672	46.08%	5.595%
15	10.709	748	750	754	rVB	36410	58428	2.21%	0.268%
16	11.155	787	789	790	rBV	36679	37638	1.42%	0.173%
17	11.292	799	801	803	rBV	647136	695017	26.28%	3.191%
18	11.578	821	826	833	rVB	24751	33886	1.28%	0.156%
19	12.698	922	924	926	rBV	113851	93348	3.53%	0.429%
20	12.881	937	940	942	rBV	2230281	2135009	80.72%	9.802%
21	13.406	984	986	988	rBV	59213	53806	2.03%	0.247%
22	13.829	1020	1023	1029	rVB	28688	75705	2.86%	0.348%
23	13.944	1031	1033	1036	rBV	629878	589190	22.28%	2.705%
24	14.435	1072	1076	1079	rBV	19984	29771	1.13%	0.137%
25	14.755	1101	1104	1106	rBV	24084	31182	1.18%	0.143%
26	14.824	1107	1110	1113	rVV	67827	70397	2.66%	0.323%
27	15.407	1159	1161	1168	rBV	329940	507356	19.18%	2.329%
28	16.298	1237	1239	1246	rVB2	12463	35701	1.35%	0.164%

Sum of corrected areas: 21780407

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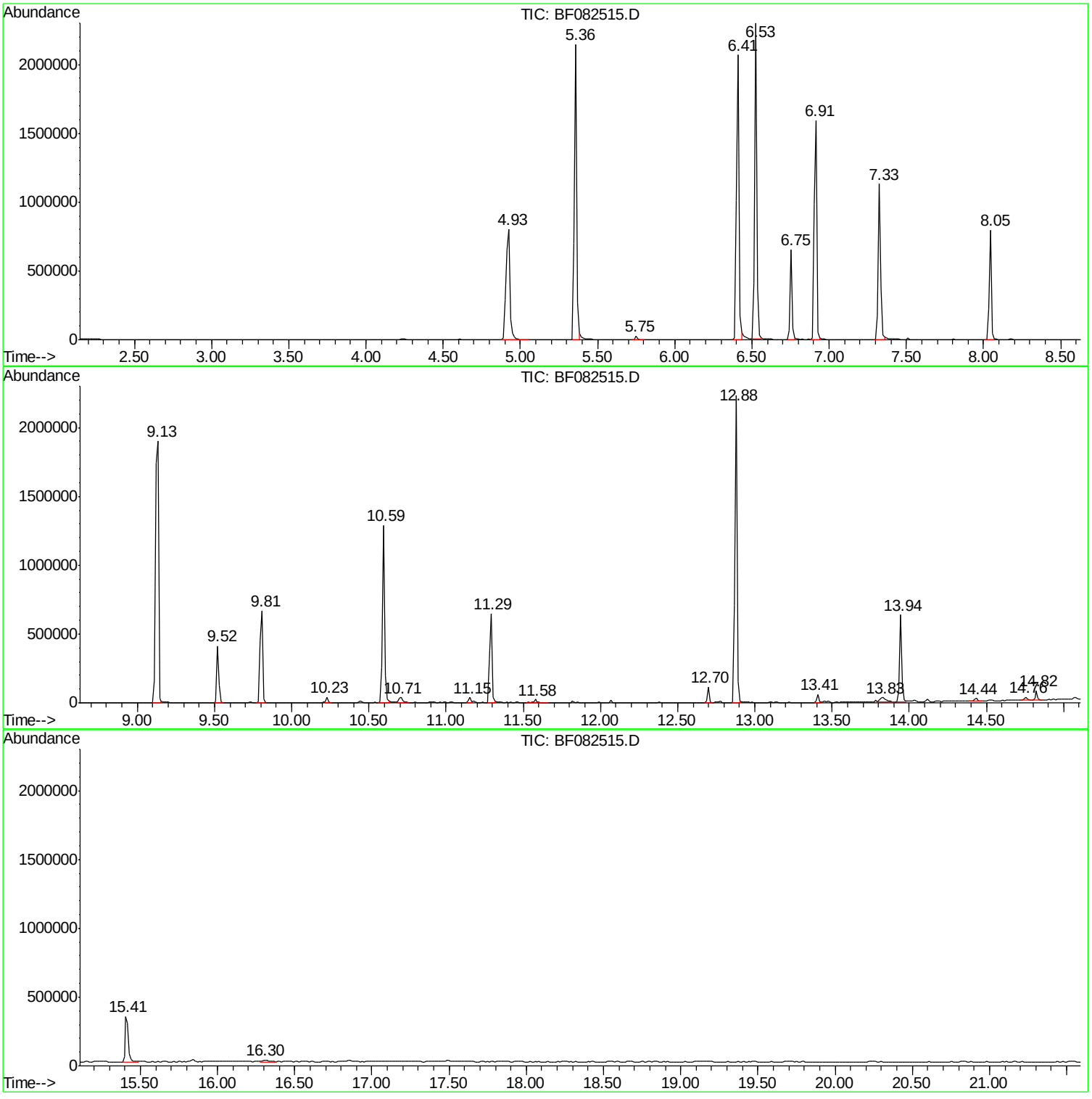
ClientSampleId :
COFF-03(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082515.D
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ClientSampleId : COFF-03(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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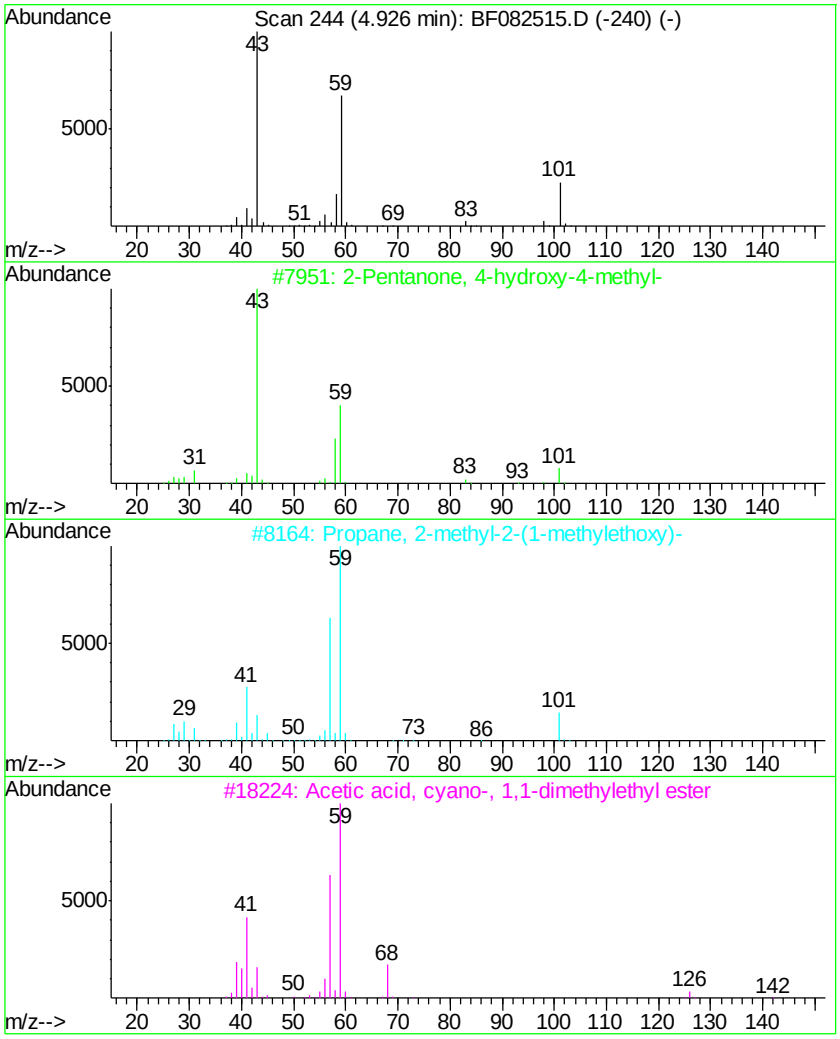
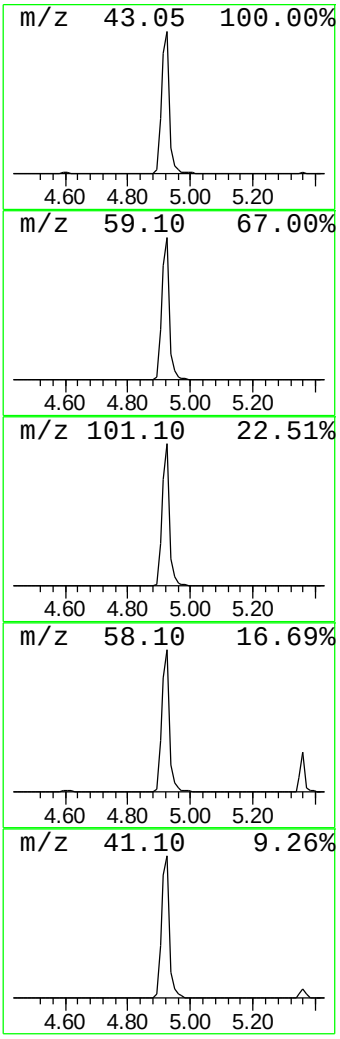
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	48.90 ng	1367280	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





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Instrument : BNA_F
ClientSampleId : COFF-03(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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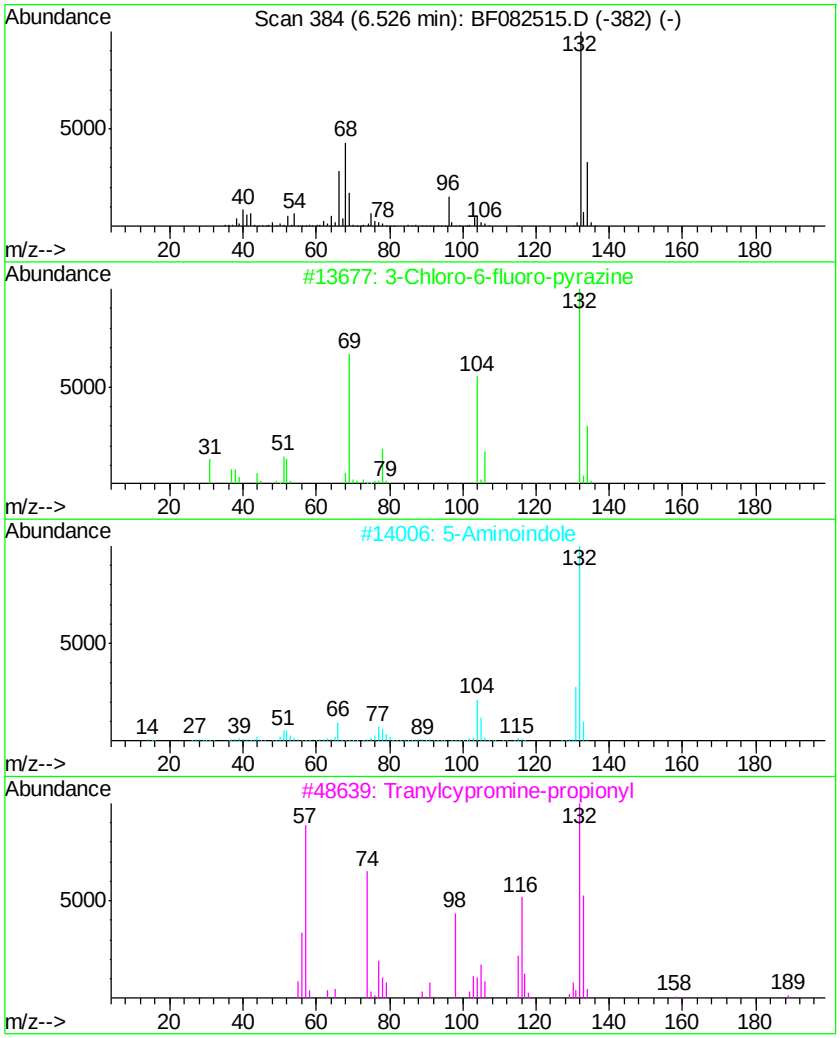
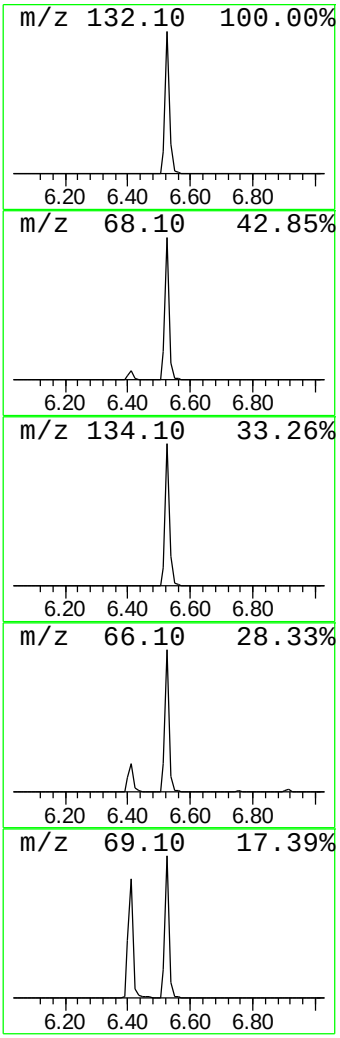
Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	76.05 ng	2126290	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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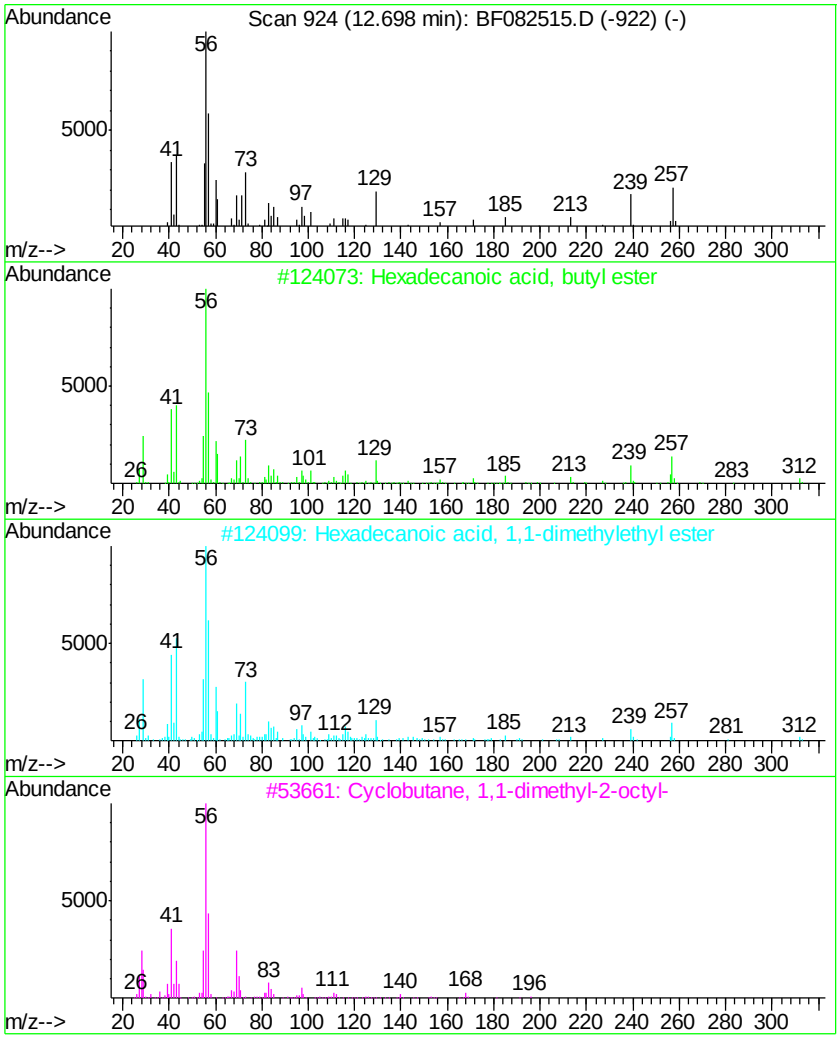
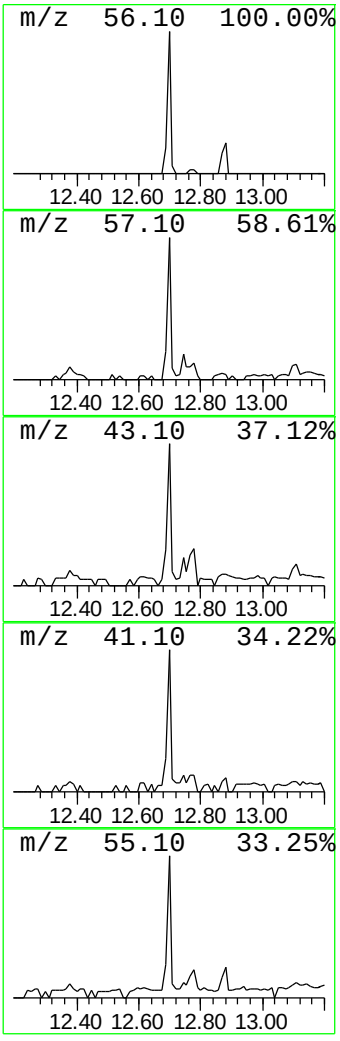
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.17 ng	93348	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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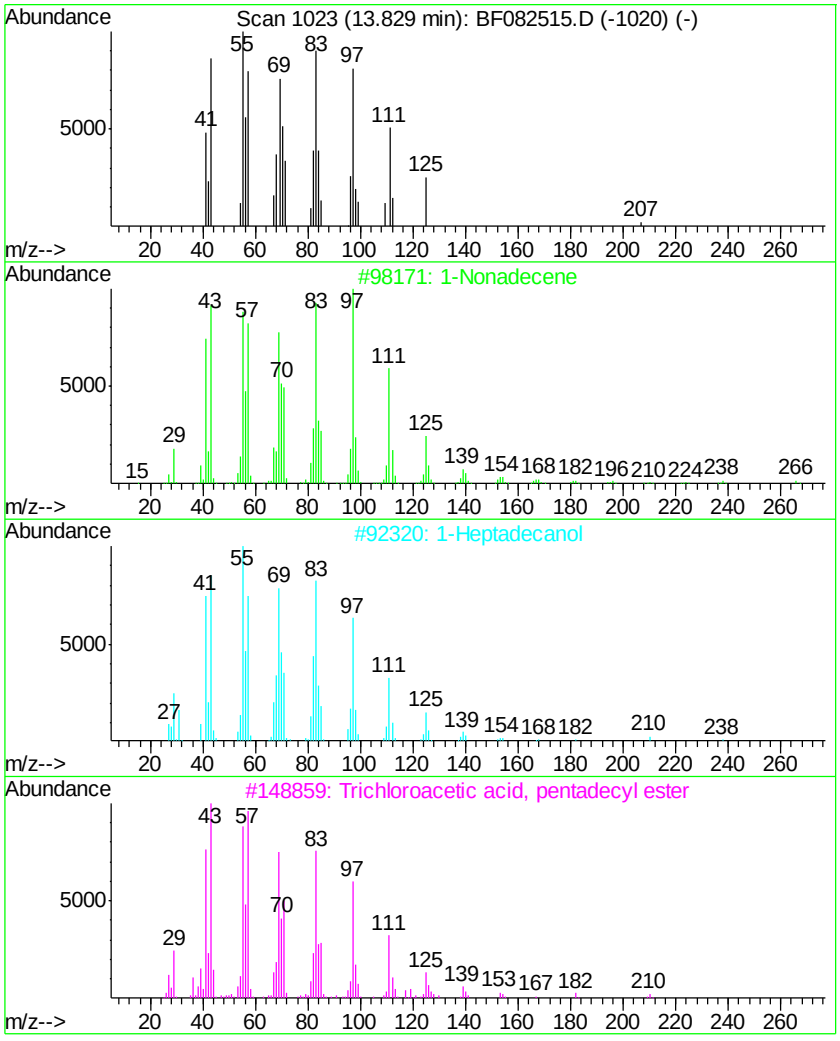
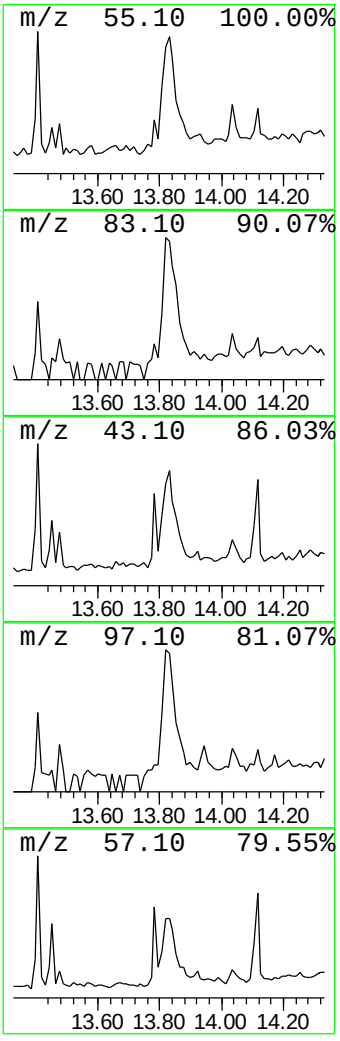
Peak Number 5 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.57 ng	75705	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	86
2	1-Heptadecanol	256	C17H36O	001454-85-9	83
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	80
4	1-Hexadecanol	242	C16H34O	036653-82-4	74
5	1-Pentadecanol	228	C15H32O	000629-76-5	74





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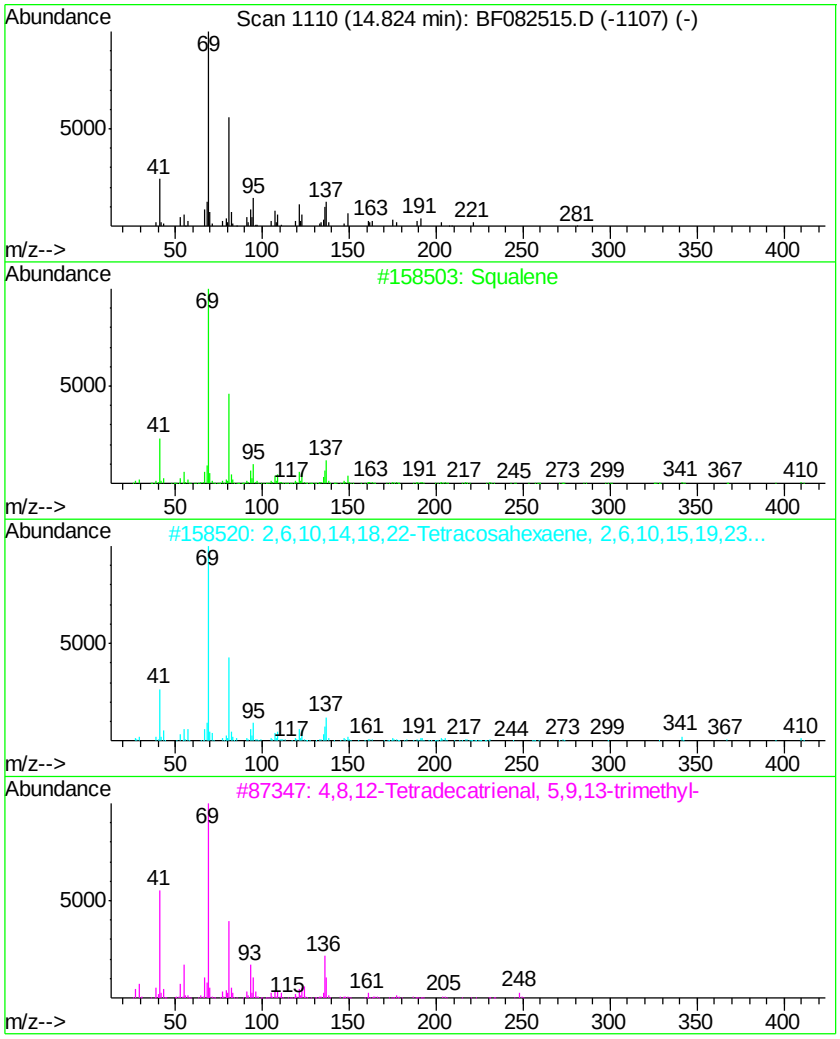
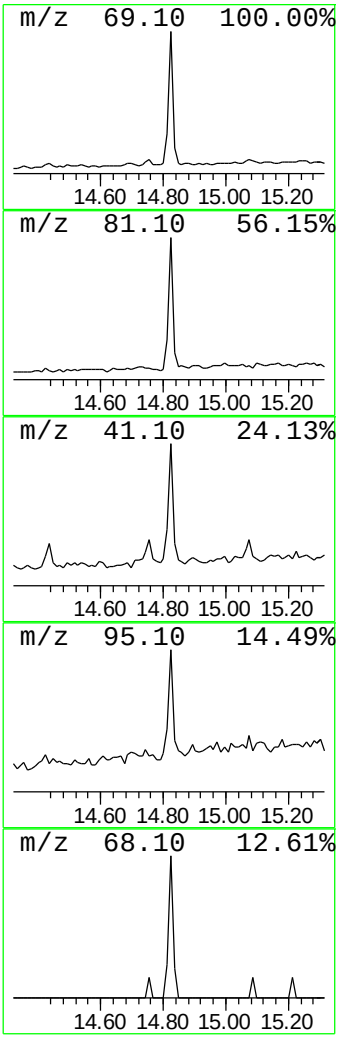
Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.78 ng	70397	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	59
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59





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...	4.93	48.9	ng	1367280	1	6.75	559165	20.0
unknown6.53	6.53	76.0	ng	2126290	1	6.75	559165	20.0
Hexadecanoic acid...	12.70	3.2	ng	93348	5	13.94	589190	20.0
1-Nonadecene	13.83	2.6	ng	75705	5	13.94	589190	20.0
Squalene	14.82	2.8	ng	70397	6	15.41	507356	20.0