LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\
Data File : BF107445.D
Acq On : 17 Jul 2018 13:21
Operator : JU/SJ
Sample : J3819-07 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-071318-D

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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	5.207	484	488	493	rVB	211847	211021	11.16%	0.928%
2	5.601	551	555	559	rBV	1716884	1488958	78.78%	6.549%
3	6.601	721	725	728	rBV	1803135	1537147	81.33%	6.761%
4	6.748	746	750	754	rBV	1775597	1594418	84.36%	7.012%
5	6.801	756	759	763	rVB2	35906	34158	1.81%	0.150%
6	6.984	786	790	793	rBV	1138827	912025	48.25%	4.011%
7	7.137	812	816	820	rBV	1514307	1240304	65.62%	5.455%
8	7.543	881	885	888	rBV	1194285	971980	51.43%	4.275%
9	8.266	1004	1008	1011	rBV	1401074	1139428	60.29%	5.011%
10	9.337	1186	1190	1194	rBV	2014470	1796055	95.03%	7.899%
11	9.442	1205	1208	1212	rBV4	24630	26210	1.39%	0.115%
12	9.731	1254	1257	1260	rVB	287168	216928	11.48%	0.954%
13	9.936	1286	1292	1295	rBV5	22408	29793	1.58%	0.131%
14	10.025	1303	1307	1311	rBV2	1428284	1287081	68.10%	5.661%
15	10.060	1311	1313	1315	rVB	63556	50222	2.66%	0.221%
16	10.231	1339	1342	1345	rVB3	30448	29186	1.54%	0.128%
17	10.572	1397	1400	1403	rVB2	48951	50735	2.68%	0.223%
18	10.813	1437	1441	1448	rBV	1285472	1160563	61.40%	5.104%
19	10.919	1453	1459	1460	rBV6	25266	35810	1.89%	0.157%
20	10.931	1460	1461	1464	rVB3	33242	25489	1.35%	0.112%
21	10.983	1464	1470	1472	rBV5	18259	32432	1.72%	0.143%
22	11.207	1505	1508	1511	rBV4	23542	30389	1.61%	0.134%
23	11.519	1557	1561	1564	rBV	1630928	1443626	76.38%	6.349%
24	11.542	1564	1565	1568	rVV	283538	158442	8.38%	0.697%
25	11.589	1571	1573	1576	rVB	63555	58640	3.10%	0.258%
26	11.748	1597	1600	1603	rVB4	41965	44088	2.33%	0.194%
27	11.854	1615	1618	1621	rBV5	21602	24919	1.32%	0.110%
28	11.895	1621	1625	1628	rBV	272685	232421	12.30%	1.022%
29	12.025	1644	1647	1649	rBV4	86773	99866	5.28%	0.439%
30	12.048	1649	1651	1654	rVB3	48711	46566	2.46%	0.205%
31	12.130	1662	1665	1668	rBV4	54391	68612	3.63%	0.302%
32	12.207	1673	1678	1681	rBV7	25303	45920	2.43%	0.202%
33	12.313	1694	1696	1700	rBV5	24503	38820	2.05%	0.171%
34	12.583	1738	1742	1743	rBV2	425905	355294	18.80%	1.563%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.607	1743	1746	1752	rVB	797843	845762	44.75%	3.720%
36	12.689	1757	1760	1764	rVB	289338	240450	12.72%	1.058%
37	12.736	1764	1768	1771	rBV	301633	288818	15.28%	1.270%
38	12.889	1792	1794	1796	rVB2	49538	24707	1.31%	0.109%
39	12.966	1802	1807	1810	rBV	280879	306313	16.21%	1.347%
40	13.101	1826	1830	1833	rBV	2071475	1890048	100.00%	8.313%
41	13.395	1877	1880	1882	rBV4	58949	71577	3.79%	0.315%
42	13.983	1978	1980	1984	rVB5	117945	110301	5.84%	0.485%
43	14.166	2007	2011	2014	rBV	1349009	1377689	72.89%	6.059%
44	15.707	2269	2273	2278	rVB2	818400	1063606	56.27%	4.678%

Sum of corrected areas: 22736817

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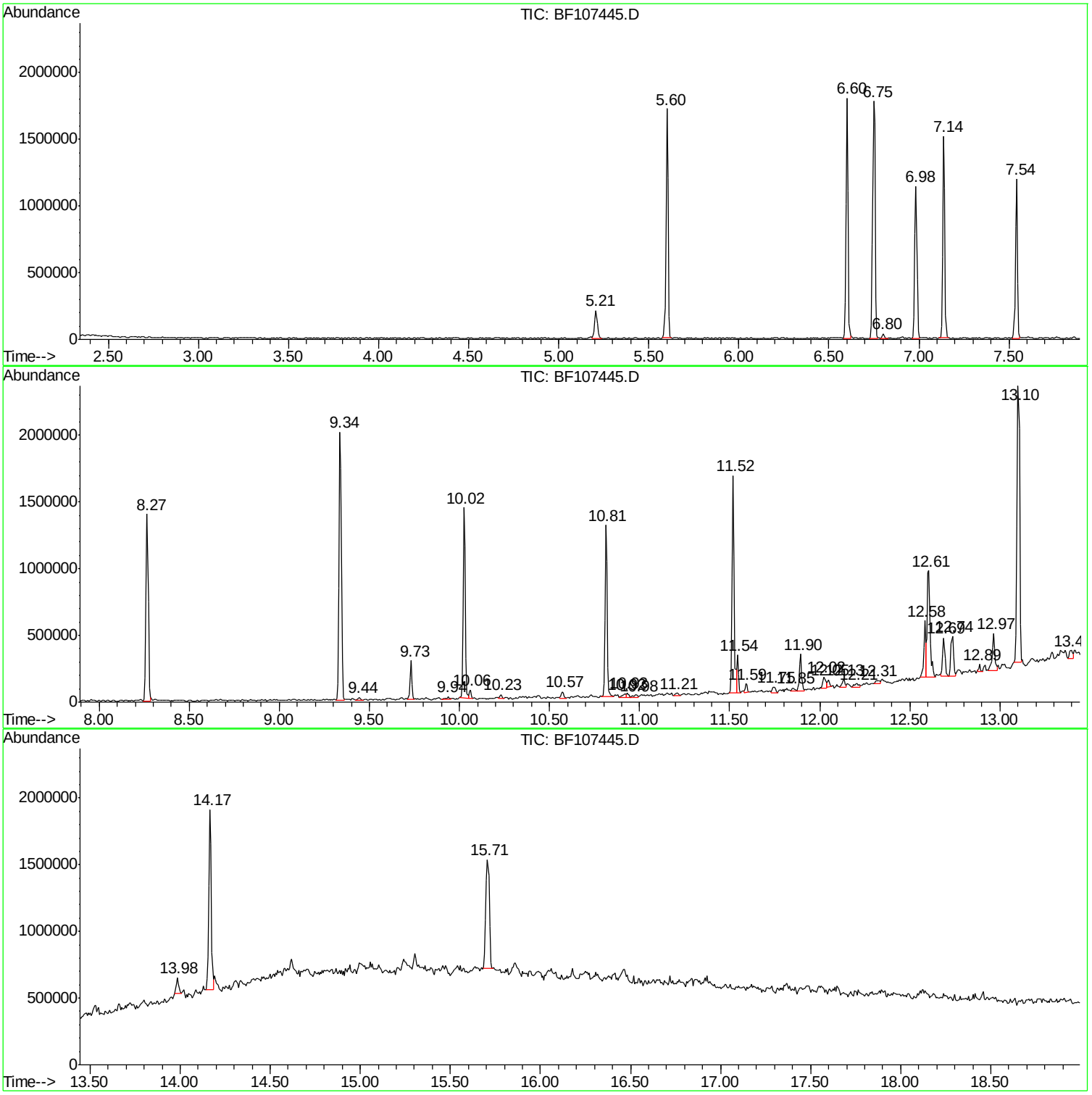
Instrument :
BNA_F
ClientSampleId :
AU-05-071318-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\
Data File : BF107445.D
Acq On : 17 Jul 2018 13:21
Operator : JU/SJ
Sample : J3819-07 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-071318-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

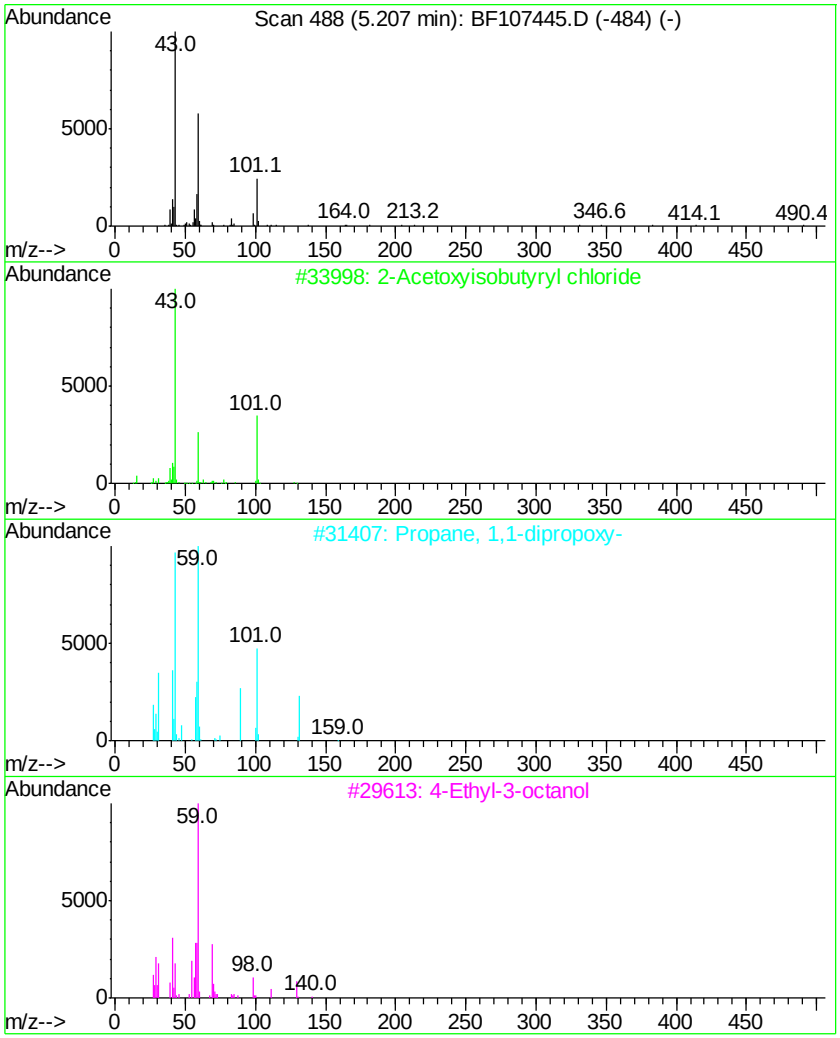
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

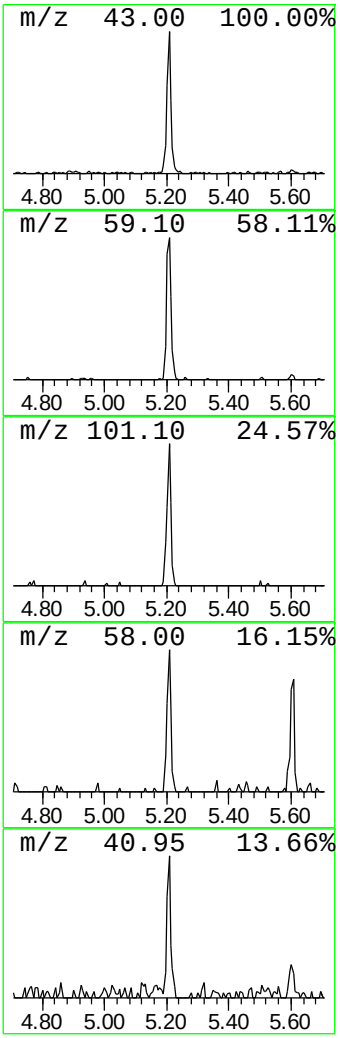
****

Peak Number 1 2-Acetoxyisobutyryl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	4.63 ng	211021	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	50
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
3	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	35
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	22
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	17





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Instrument : BNA_F
ClientSampleId : AU-05-071318-D

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TIC Library : C:\DATABASE\NIST11.L
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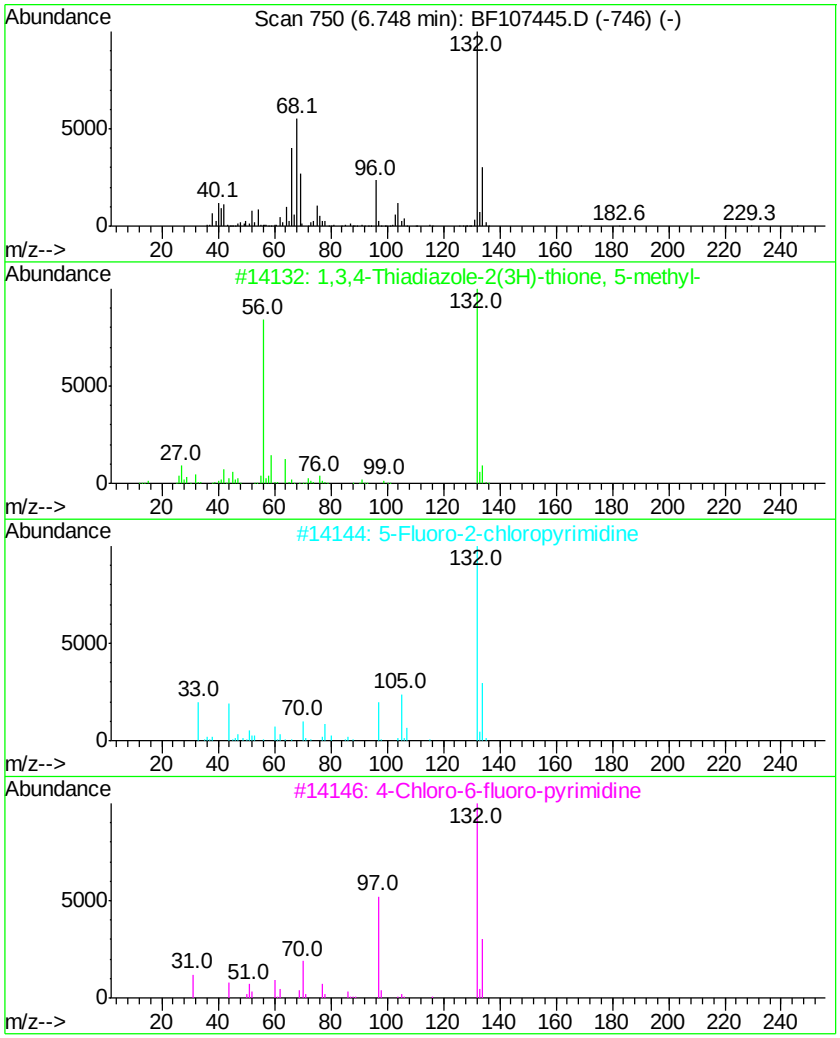
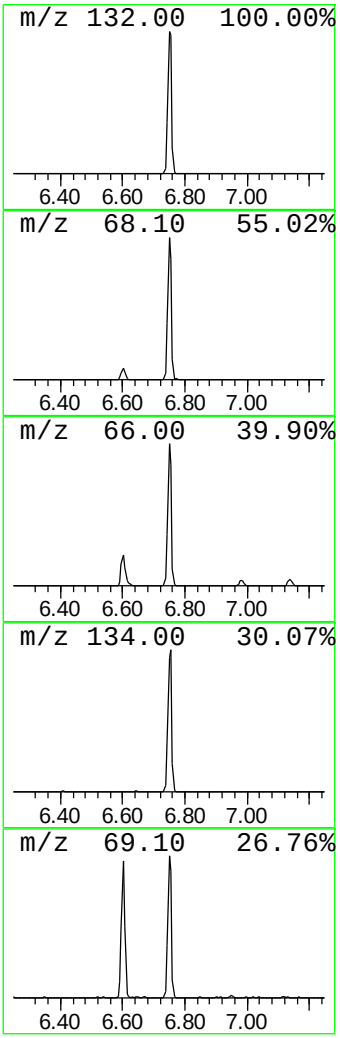
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	34.96 ng	1594420	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
5	1H-Indenol	132	C9H8O	056631-57-3	10





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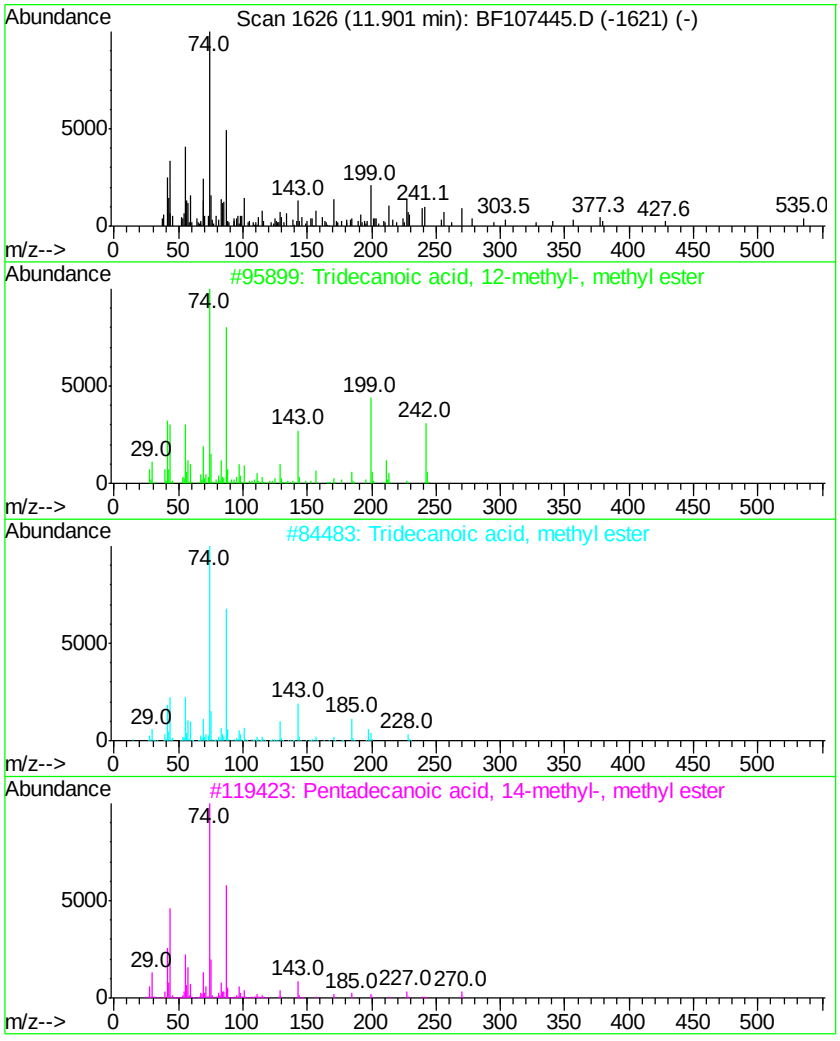
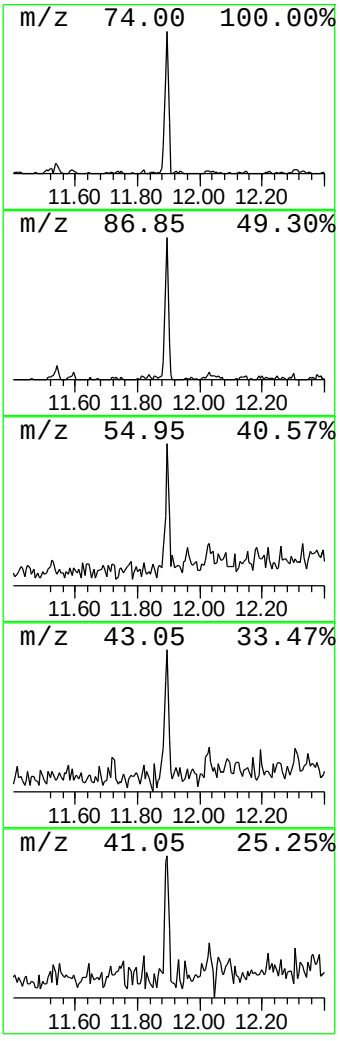
Peak Number 4 Tridecanoic acid, 12-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.22 ng	232421	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	83
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	83
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	80





Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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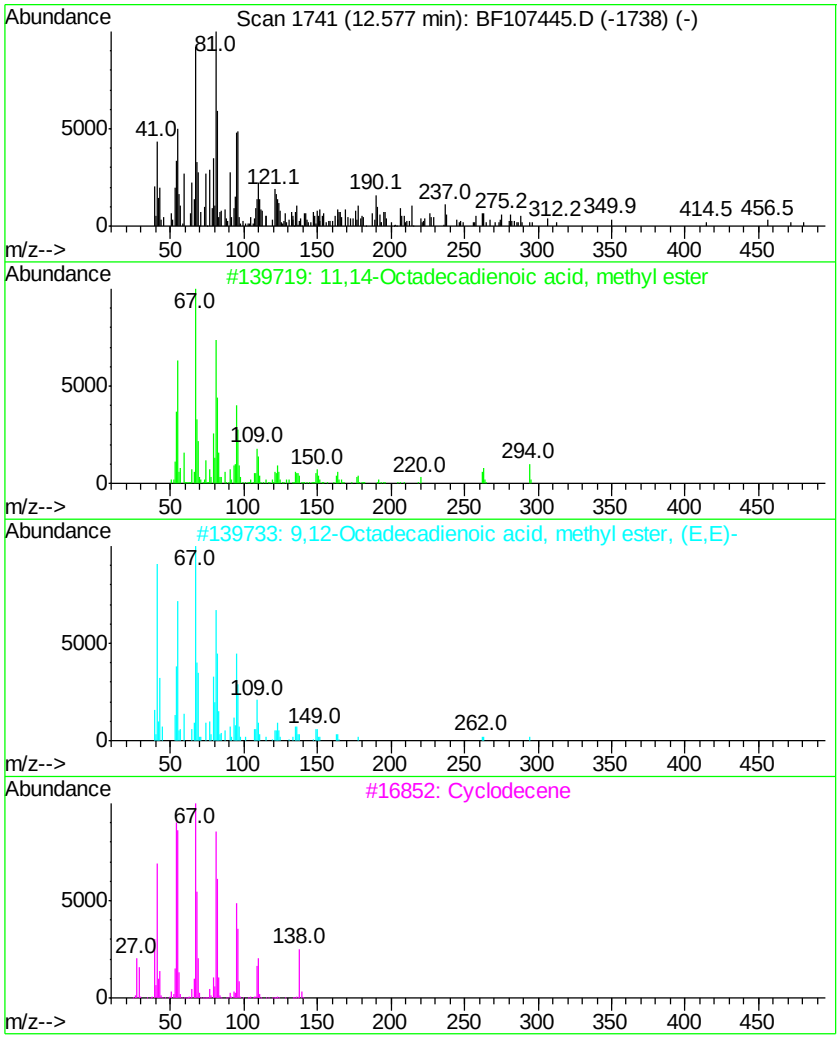
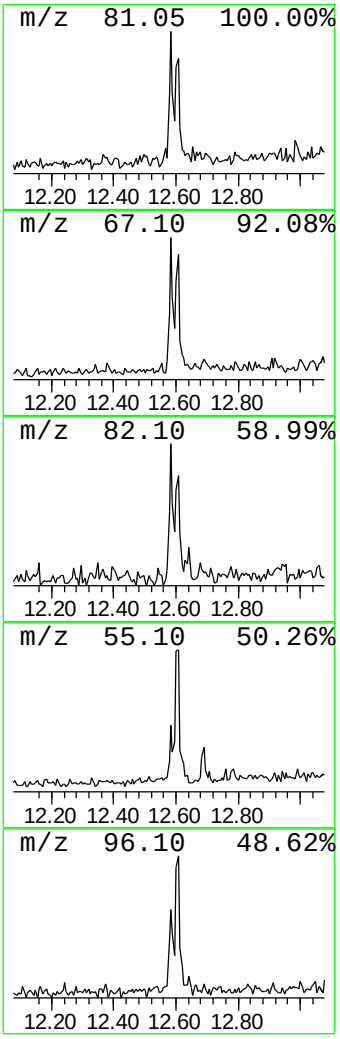
Peak Number 5 11,14-Octadecadienoic acid,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	4.92 ng	355294	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	95
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	93
3	Cyclodecene	138	C10H18	003618-12-0	91
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	91
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	78





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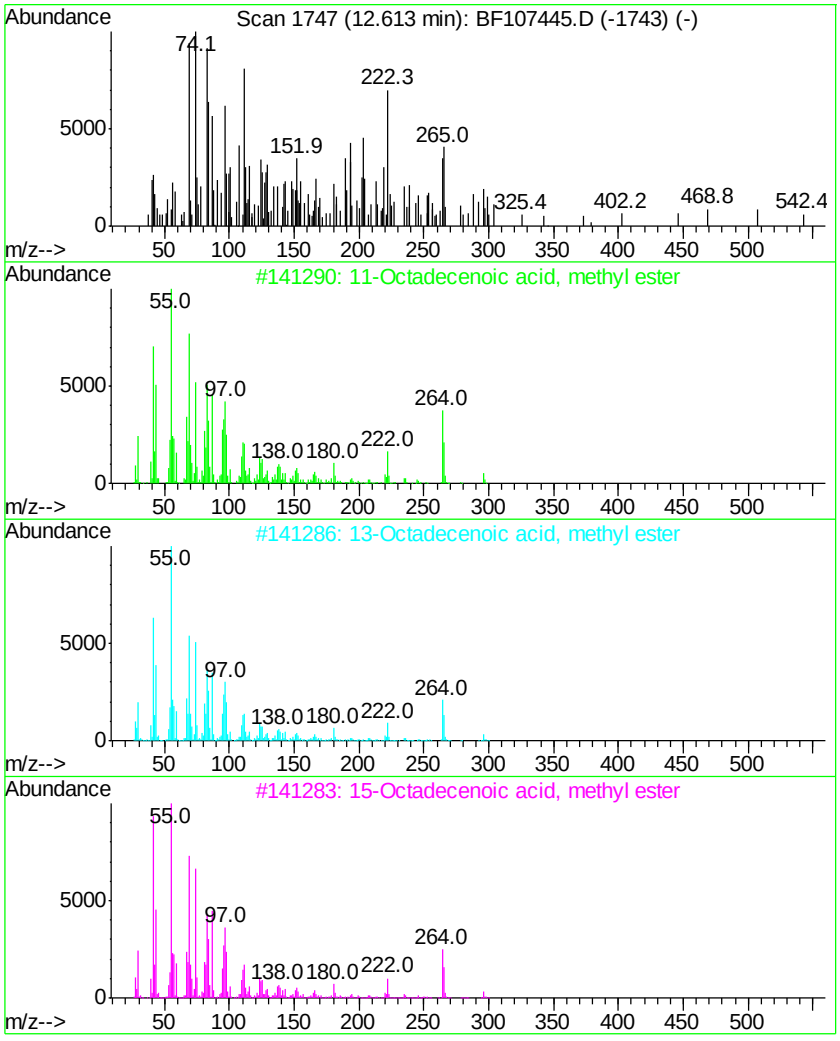
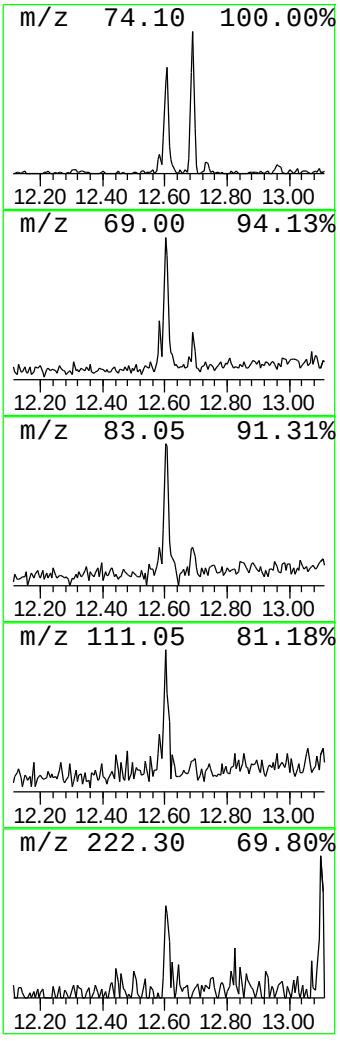
Peak Number 6 11-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	11.72 ng	845762	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	93
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	87





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Acetoxyisobutyr...	5.21	4.6	ng	211021	1	6.98	912025	20.0
unknown6.75	6.75	35.0	ng	1594420	1	6.98	912025	20.0
Tridecanoic acid,...	11.90	3.2	ng	232421	4	11.52	1443630	20.0
11,14-Octadecadie...	12.58	4.9	ng	355294	4	11.52	1443630	20.0
11-Octadecenoic a...	12.61	11.7	ng	845762	4	11.52	1443630	20.0