LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096543.D
Acq On : 6 Jul 2017 19:48
Operator : SJ/MA
Sample : I3972-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B2-18.5-19

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-BF070117.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	4.910	475	480	490	rVB	287803	401919	15.09%	1.834%
2	5.334	547	552	555	rBV	2706639	2631450	98.81%	12.010%
3	6.357	720	726	730	rBV	2549034	2663253	100.00%	12.155%
4	6.487	743	748	751	rBV	2759066	2569754	96.49%	11.729%
5	6.716	783	787	790	rBV	734481	650795	24.44%	2.970%
6	6.869	809	813	817	rBV	2017367	1909622	71.70%	8.716%
7	7.275	877	882	885	rBV	1695461	1584250	59.49%	7.231%
8	7.375	893	899	909	rVB	25729	31069	1.17%	0.142%
9	7.992	1000	1004	1008	rBV	902226	846174	31.77%	3.862%
10	9.075	1183	1188	1191	rBV	2596676	2251314	84.53%	10.275%
11	9.469	1251	1255	1258	rBV	312798	272722	10.24%	1.245%
12	9.751	1298	1303	1307	rBV	859613	784687	29.46%	3.581%
13	10.192	1375	1378	1381	rVB	53017	43409	1.63%	0.198%
14	10.416	1409	1416	1418	rBV2	20616	30255	1.14%	0.138%
15	10.533	1432	1436	1440	rBV	1166437	1153149	43.30%	5.263%
16	10.669	1455	1459	1466	rBV	69131	85350	3.20%	0.390%
17	11.116	1531	1535	1537	rBV2	51473	42598	1.60%	0.194%
18	11.233	1551	1555	1558	rBV	666569	632563	23.75%	2.887%
19	11.469	1592	1595	1603	rVB	100839	93326	3.50%	0.426%
20	12.286	1730	1734	1740	rBV	168812	165035	6.20%	0.753%
21	12.439	1756	1760	1763	rBV	68177	59044	2.22%	0.269%
22	12.668	1793	1799	1802	rBV	55661	65655	2.47%	0.300%
23	12.816	1820	1824	1828	rBV	1753877	1628502	61.15%	7.433%
24	13.721	1974	1978	1985	rBV	125992	142217	5.34%	0.649%
25	13.863	1997	2002	2005	rBV	727359	696724	26.16%	3.180%
26	15.274	2238	2242	2248	rVB	407882	475292	17.85%	2.169%

Sum of corrected areas: 21910128

LSC Report - Integrated Chromatogram

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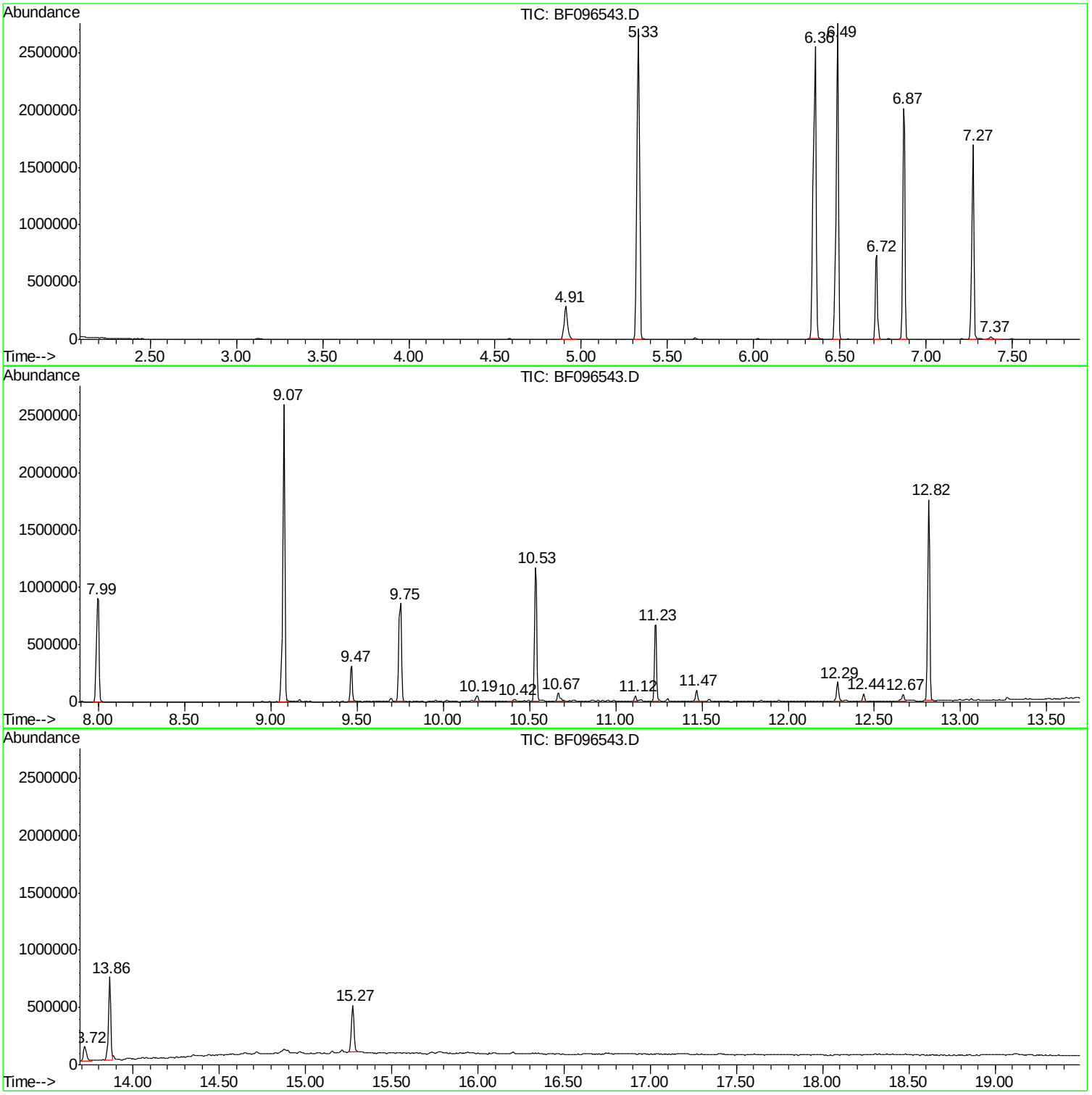
ClientSampleId :
B2-18.5-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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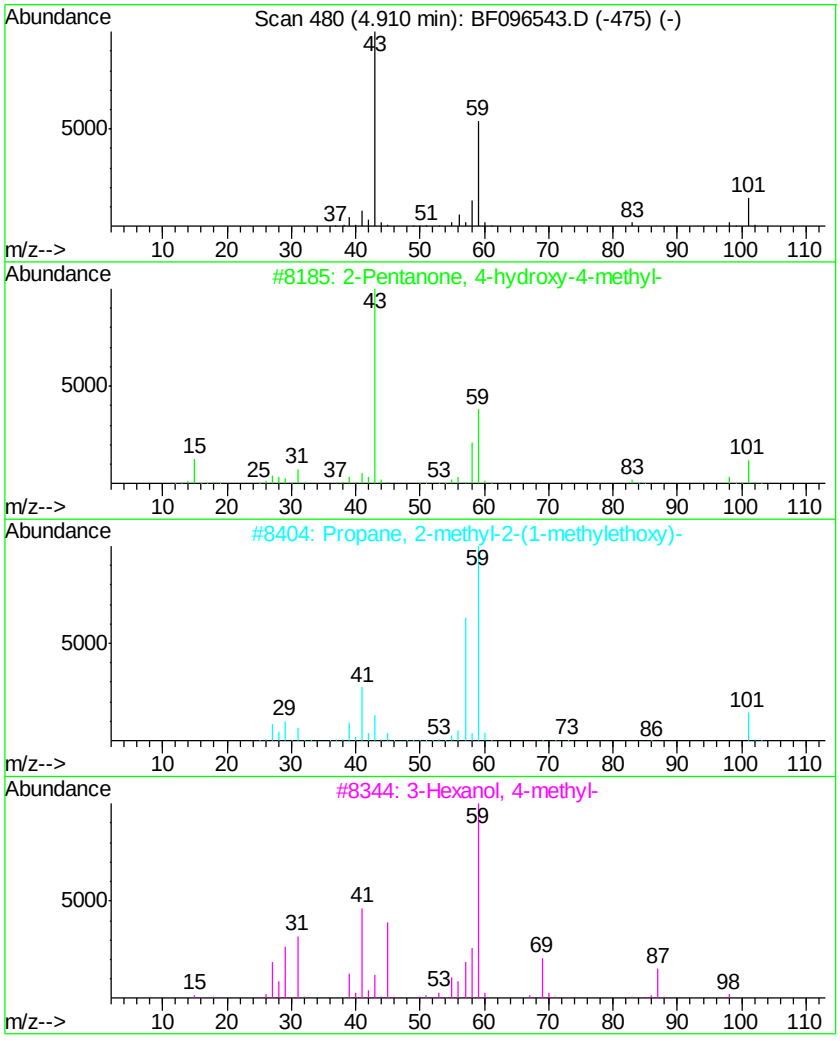
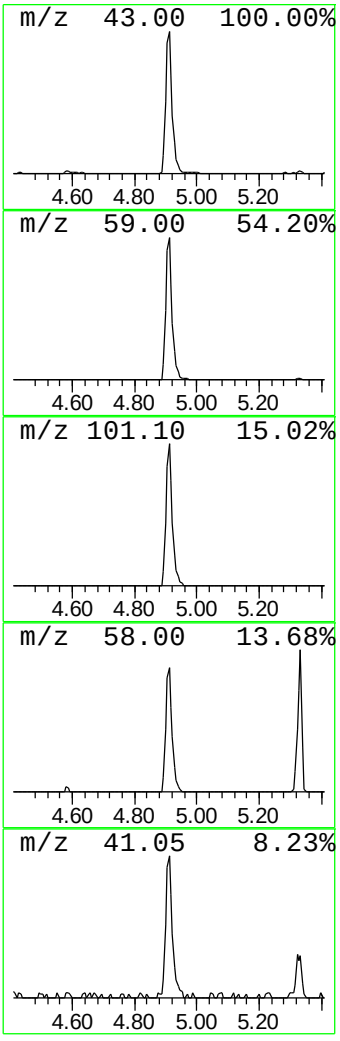
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	12.35 ng	401919	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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ClientSampleId : B2-18.5-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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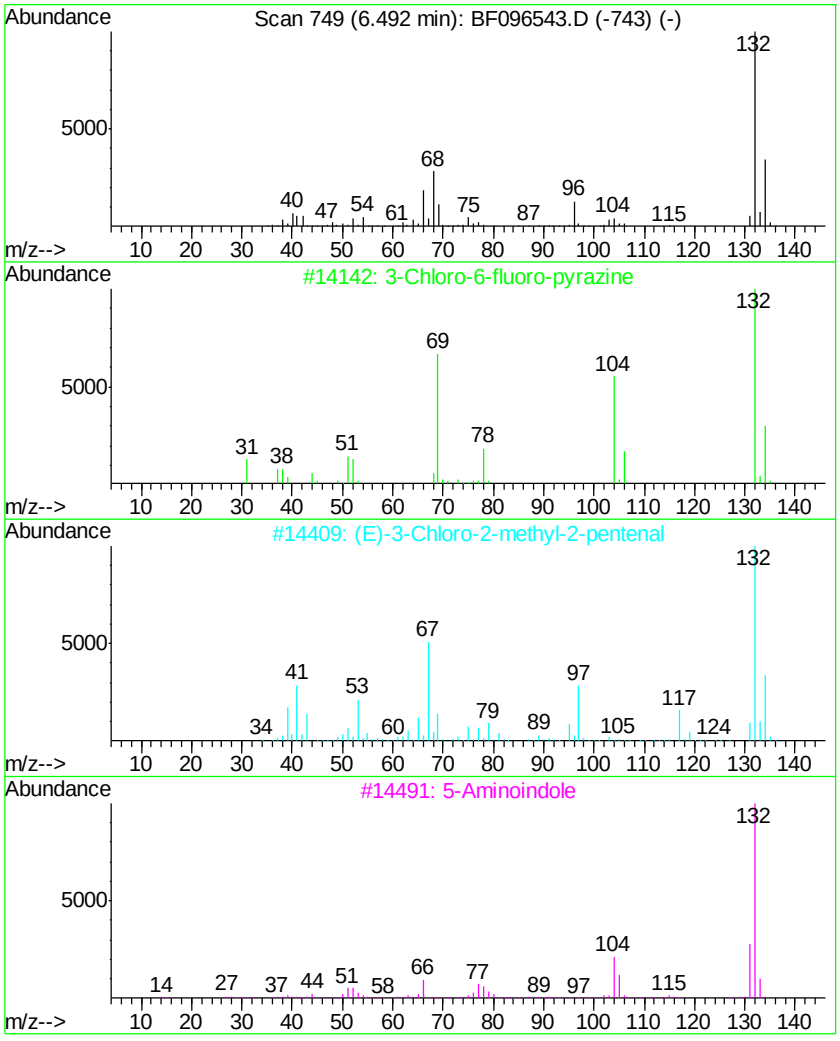
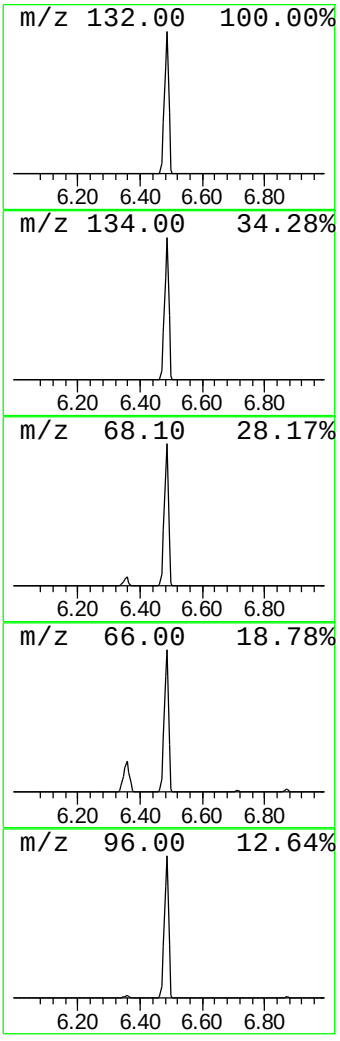
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	78.97 ng	2569750	1,4-Dichlorobenzene-d4	6.72

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Sample : I3972-02
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Instrument : BNA_F
ClientSampleId : B2-18.5-19

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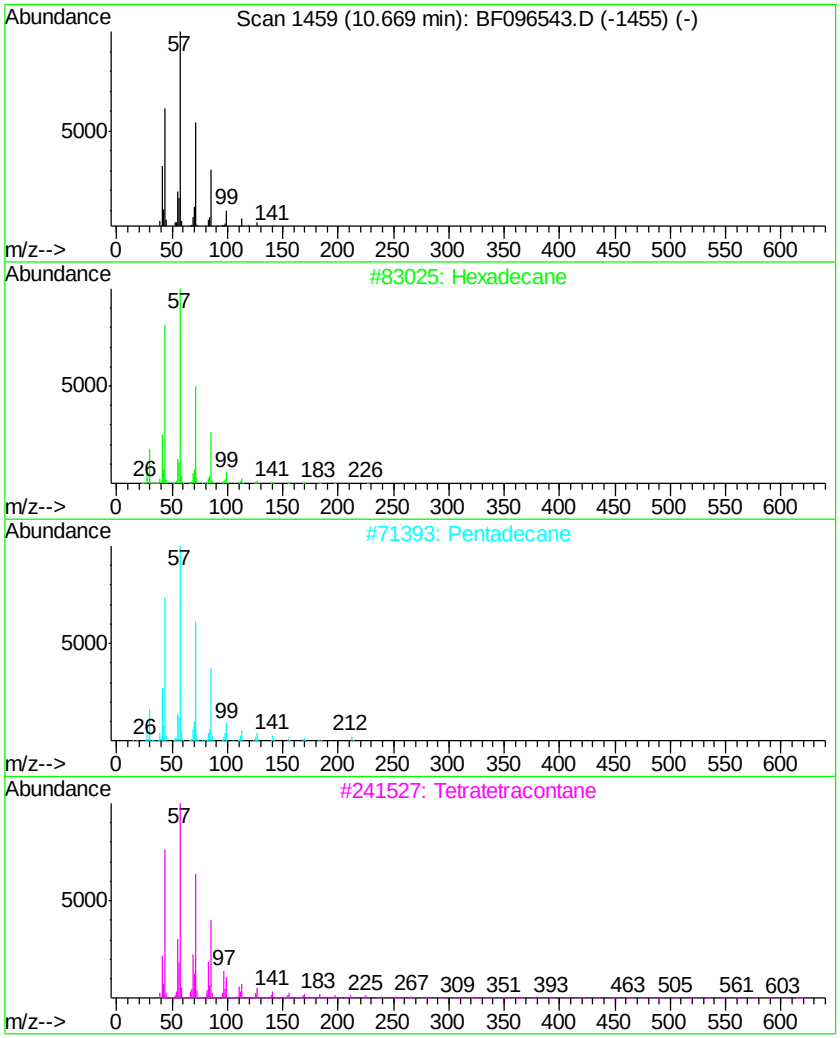
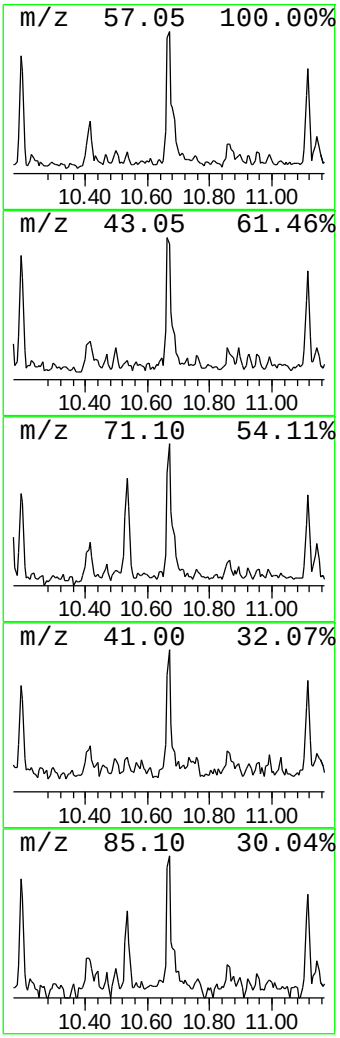
Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.70 ng	85350	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64





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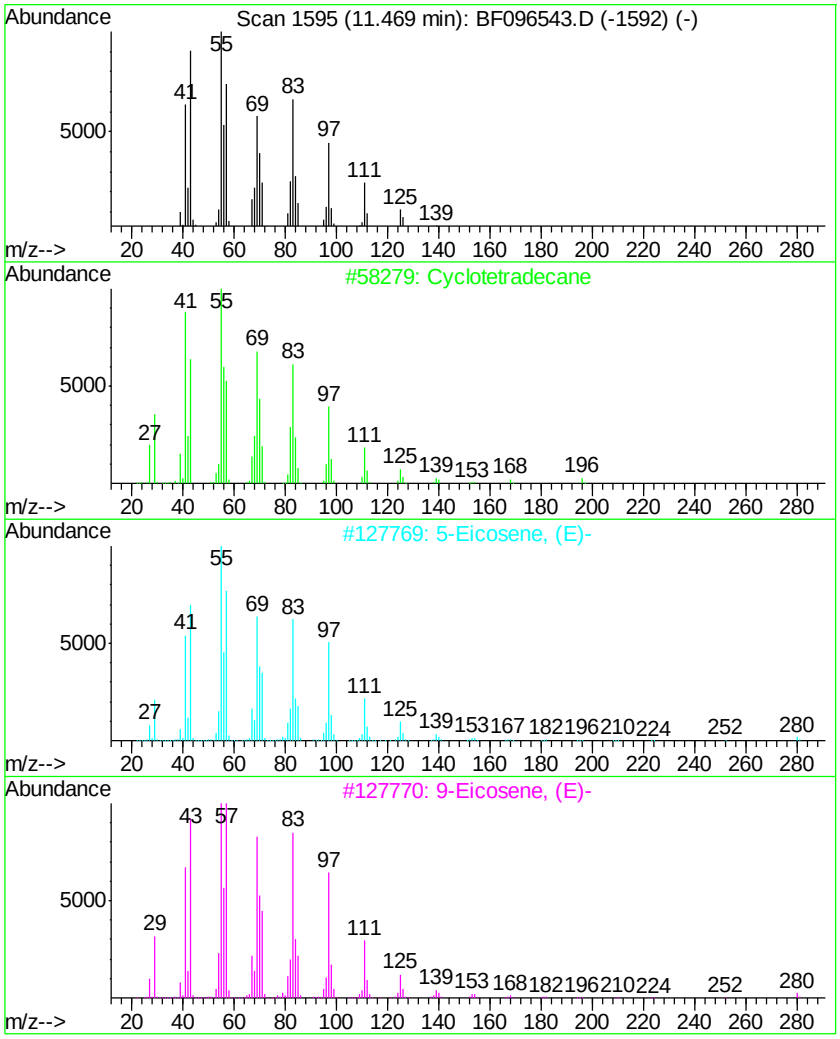
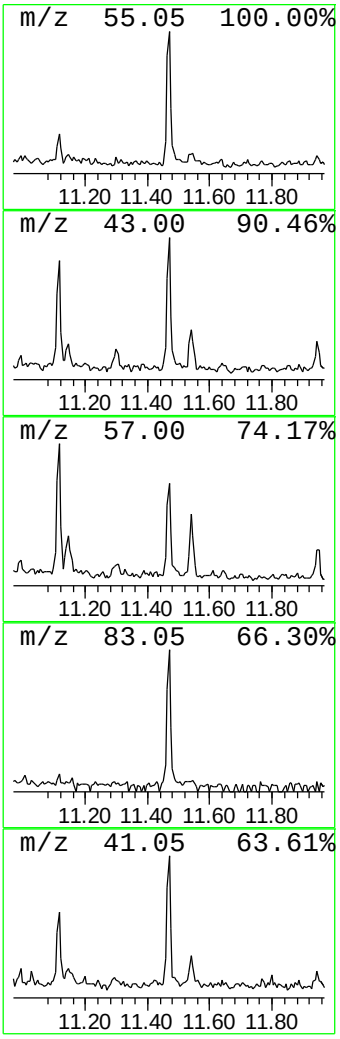
Peak Number 5 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.95 ng	93326	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	87
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	87





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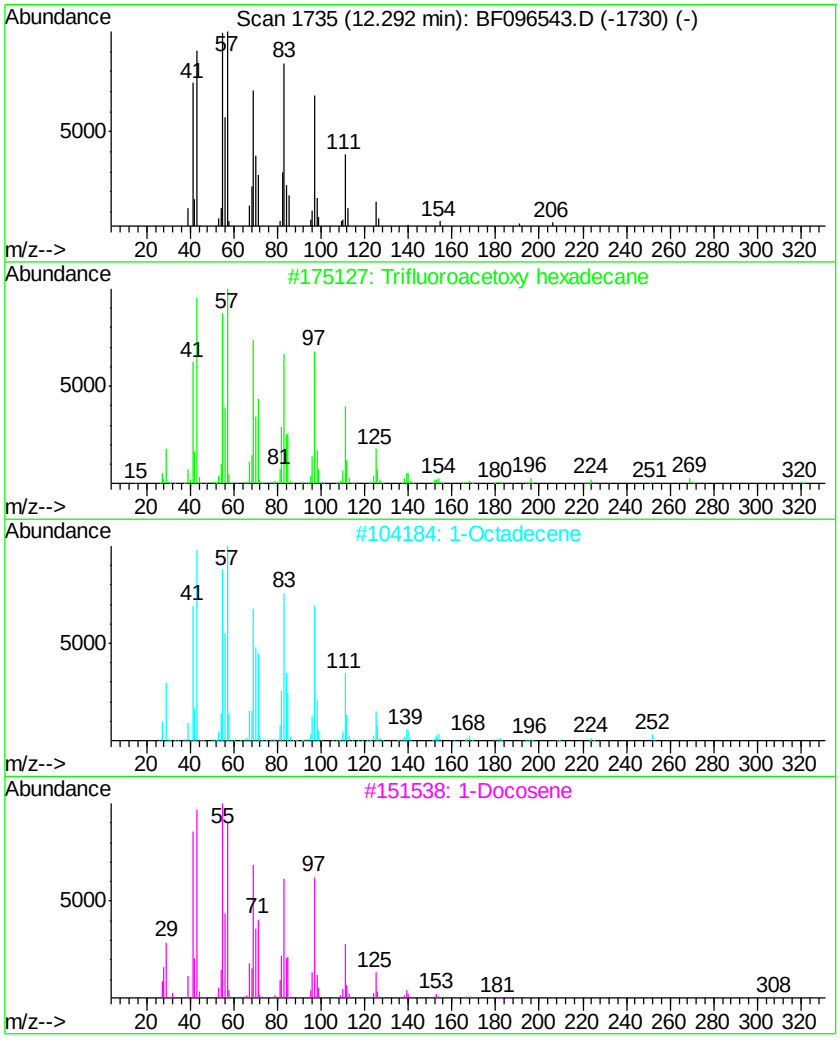
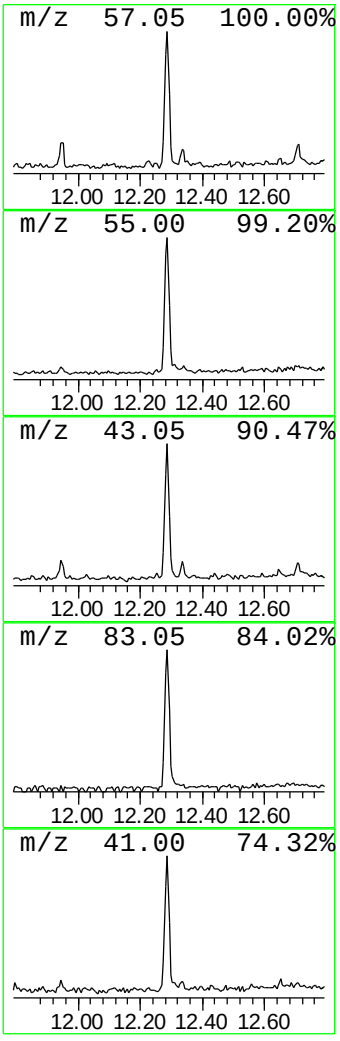
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	5.22 ng	165035	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	1-Octadecene	252	C18H36	000112-88-9	90
3	1-Docosene	308	C22H44	001599-67-3	90
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	90





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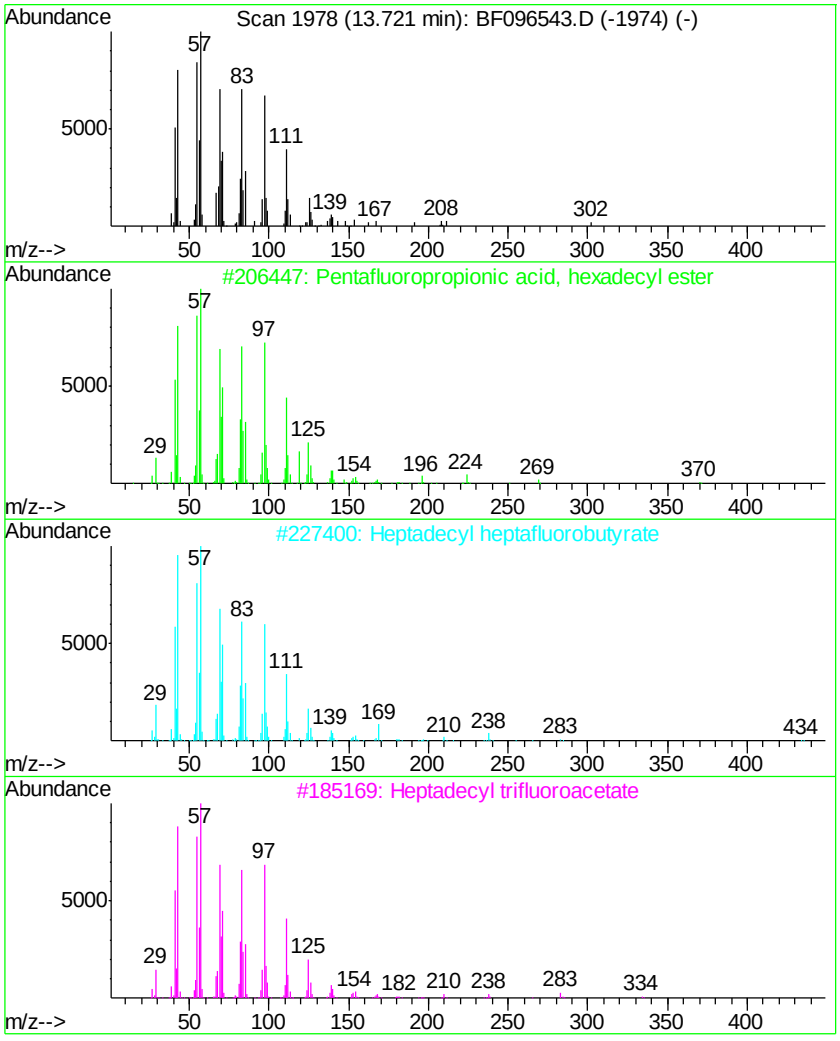
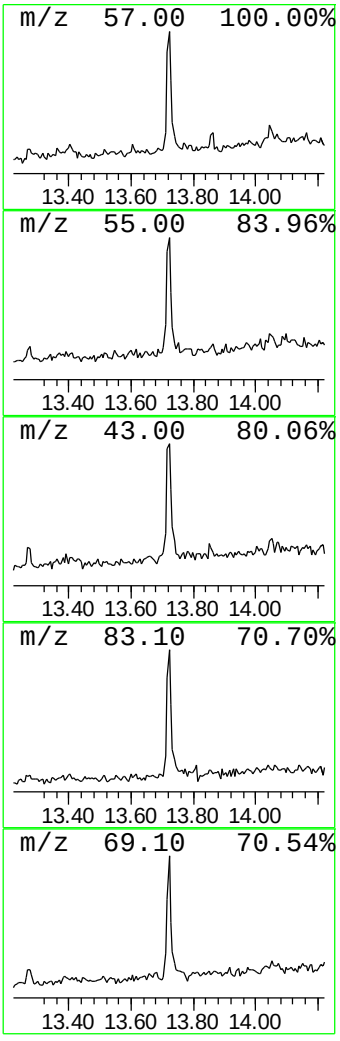
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.08 ng	142217	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	1-Docosene	308	C22H44	001599-67-3	91
5	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91





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...	4.91	12.4	ng	401919	1	6.72	650795	20.0
unknown6.49	6.49	79.0	ng	2569750	1	6.72	650795	20.0
Hexadecane	10.67	2.7	ng	85350	4	11.23	632563	20.0
Cyclotetradecane	11.47	3.0	ng	93326	4	11.23	632563	20.0
Trifluoroacetoxy ...	12.29	5.2	ng	165035	4	11.23	632563	20.0
Pentafluoropropio...	13.72	4.1	ng	142217	5	13.86	696724	20.0