LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093021\
Data File : BF125736.D
Acq On : 30 Sep 2021 16:37
Operator : JU/CG
Sample : M3986-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P287-DITCH

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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125736.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	27	rVB	3757657	5045762	81.41%	12.913%
2	2.299	31	36	44	rVB2	42223	63858	1.03%	0.163%
3	5.498	576	580	584	rBV	2230998	2143670	34.59%	5.486%
4	6.498	746	750	756	rBV	1591568	1299374	20.96%	3.325%
5	6.887	812	816	819	rBV	1464533	1203196	19.41%	3.079%
6	7.445	905	911	914	rBV	3317288	3273238	52.81%	8.377%
7	8.069	1013	1017	1026	rBV	59726	74229	1.20%	0.190%
8	8.169	1029	1034	1037	rBV	1848000	1673955	27.01%	4.284%
9	8.569	1099	1102	1105	rBV	164578	123562	1.99%	0.316%
10	8.857	1145	1151	1156	rBV2	210991	337854	5.45%	0.865%
11	9.245	1211	1217	1220	rBV	6520926	6198125	100.00%	15.862%
12	9.922	1328	1332	1335	rBV	2304347	1953742	31.52%	5.000%
13	10.710	1461	1466	1469	rBV	4039784	3838471	61.93%	9.823%
14	11.033	1516	1521	1524	rBV	84582	93491	1.51%	0.239%
15	11.404	1580	1584	1588	rBV	2518460	2056769	33.18%	5.264%
16	11.927	1669	1673	1687	rBV	483042	531662	8.58%	1.361%
17	12.716	1803	1807	1809	rBV	256737	254047	4.10%	0.650%
18	12.992	1849	1854	1857	rBV	6225226	5825954	94.00%	14.910%
19	13.898	2002	2008	2019	rBV3	89434	224305	3.62%	0.574%
20	14.039	2028	2032	2042	rVB	1723922	1520190	24.53%	3.890%
21	15.515	2277	2283	2296	rBV	1061384	1339298	21.61%	3.428%

Sum of corrected areas: 39074752

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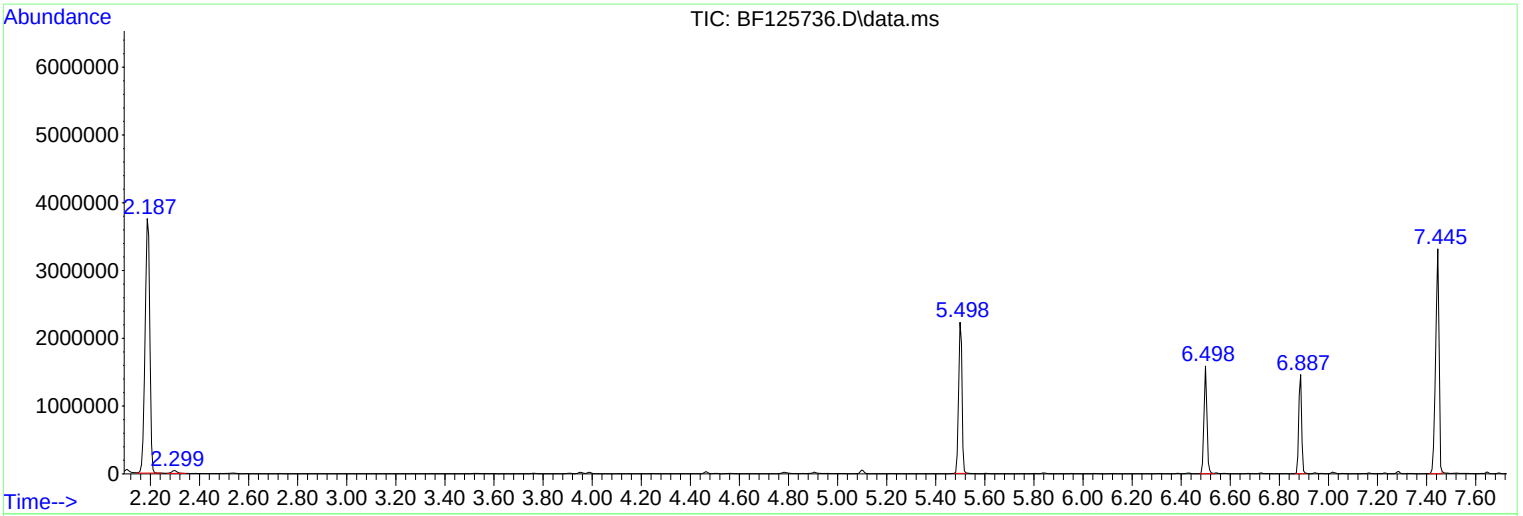
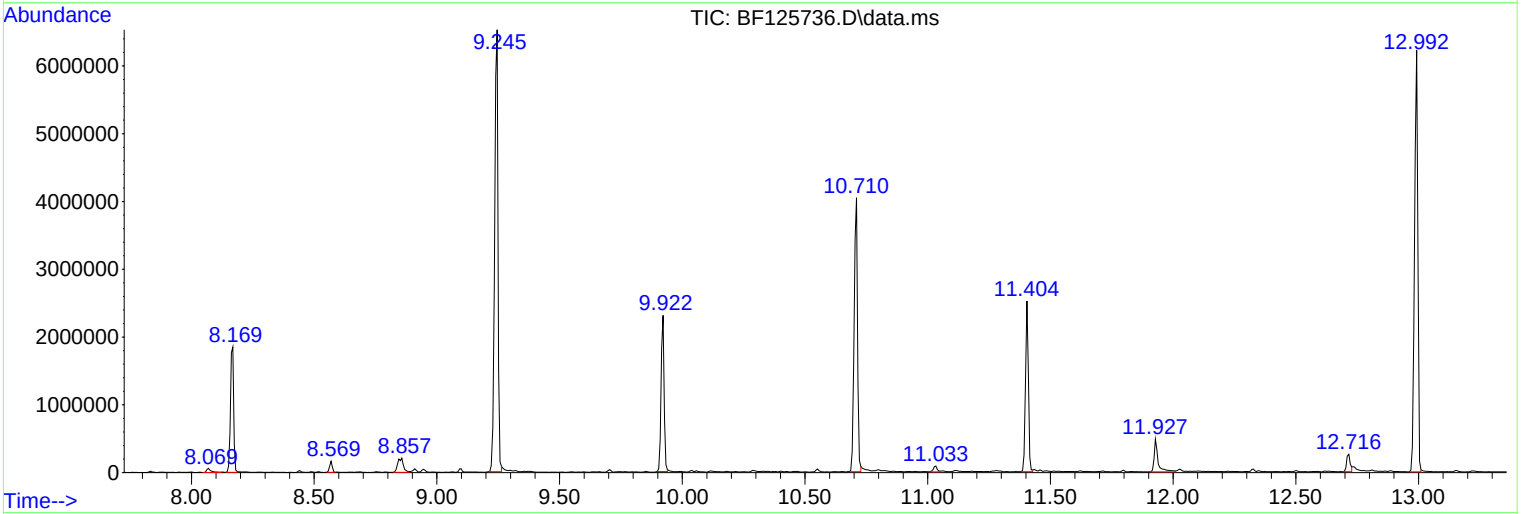
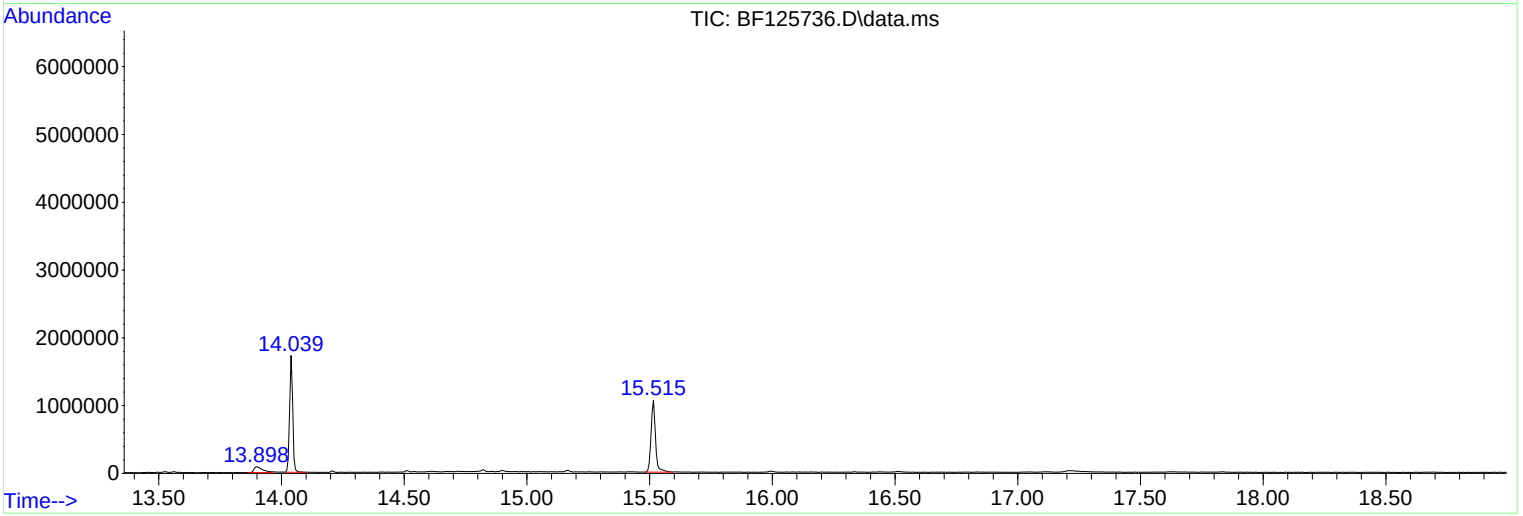
BNA_F
ClientSampleId :
P287-DITCH

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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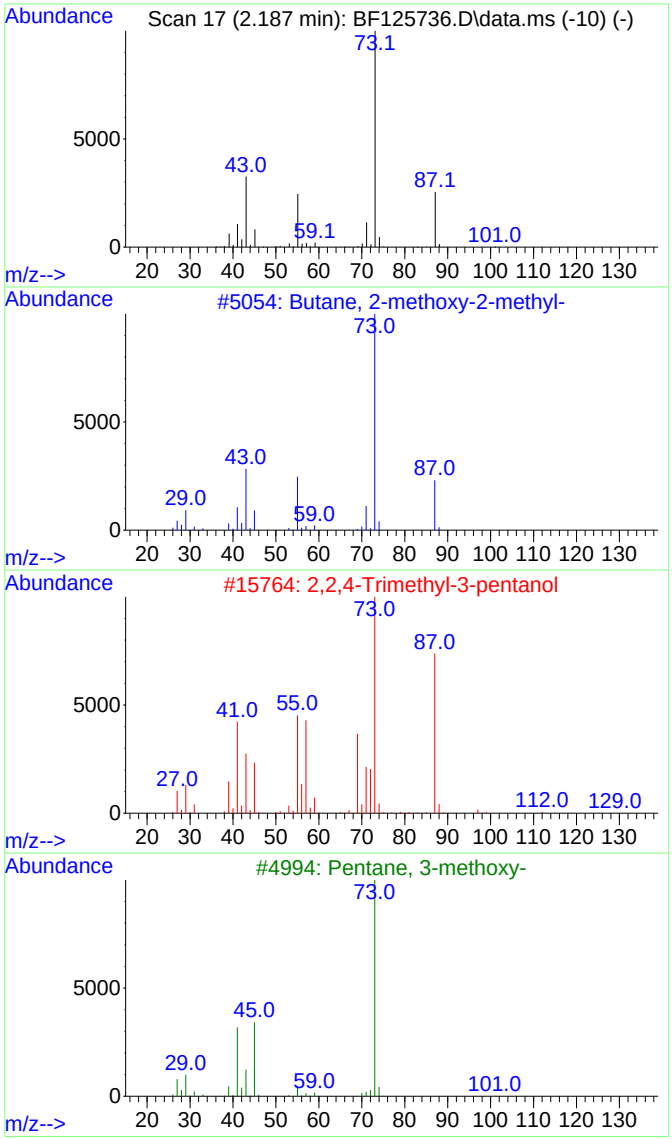
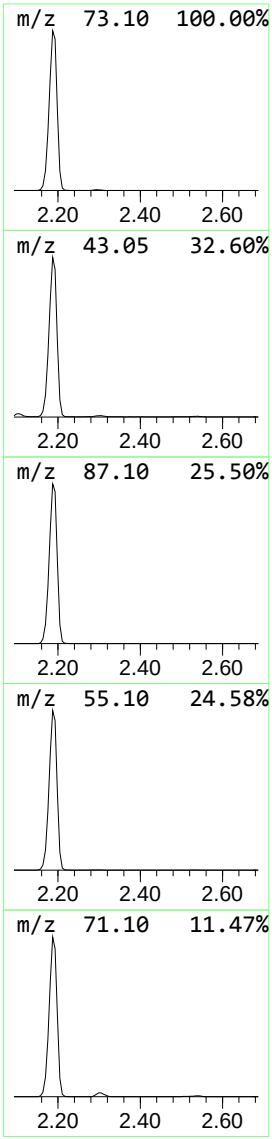
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	83.87 ng	5045760	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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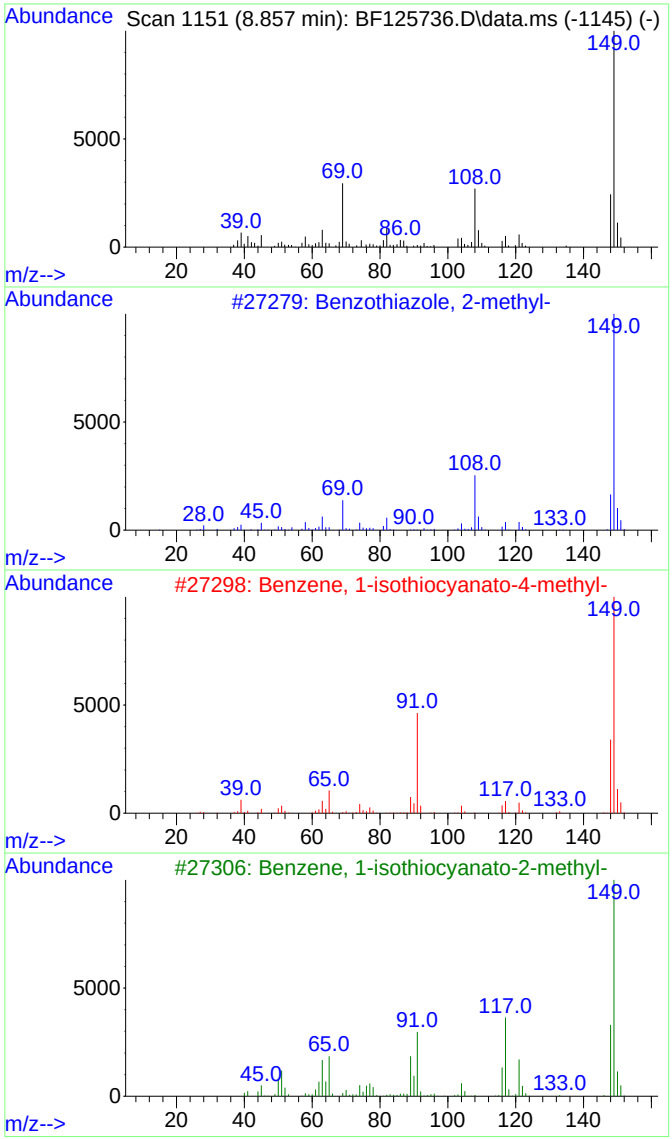
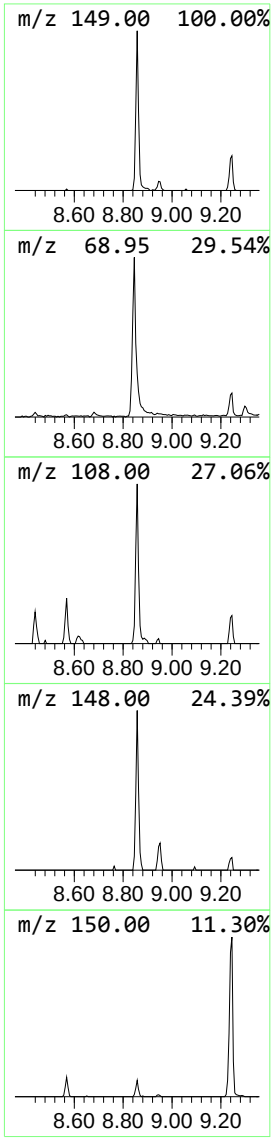
Peak Number 2 Benzothiazole, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.857	4.04 ng	337854	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	93
2	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	72
3	Benzene, 1-isothiocyanato-2-methyl-	149	C8H7NS	000614-69-7	64
4	7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	59
5	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	59





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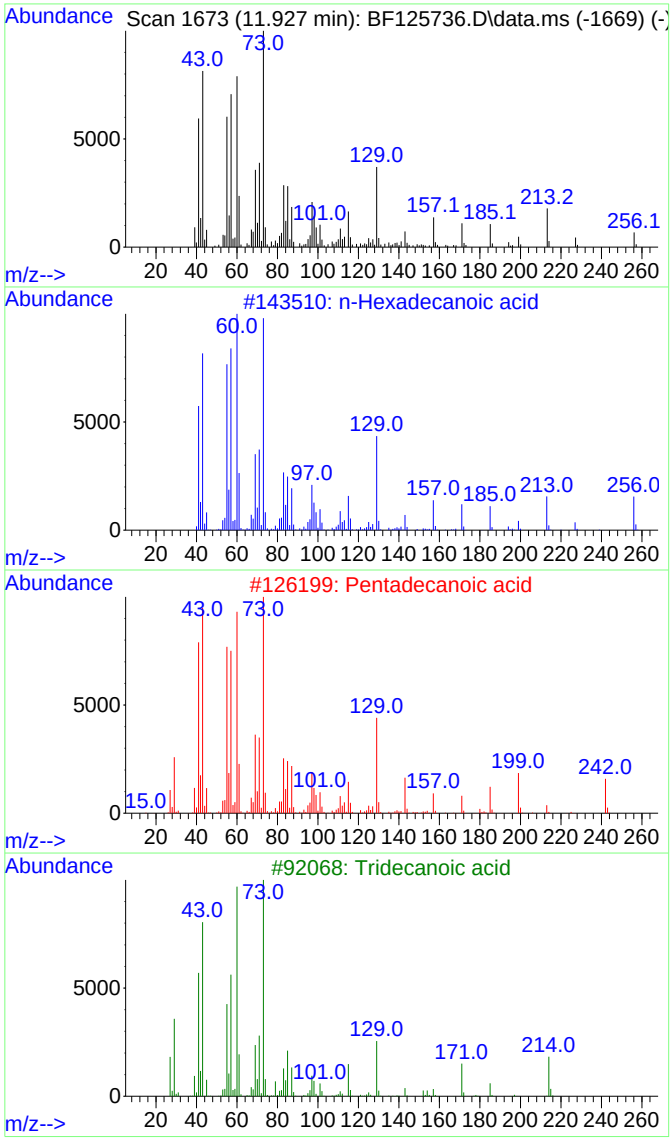
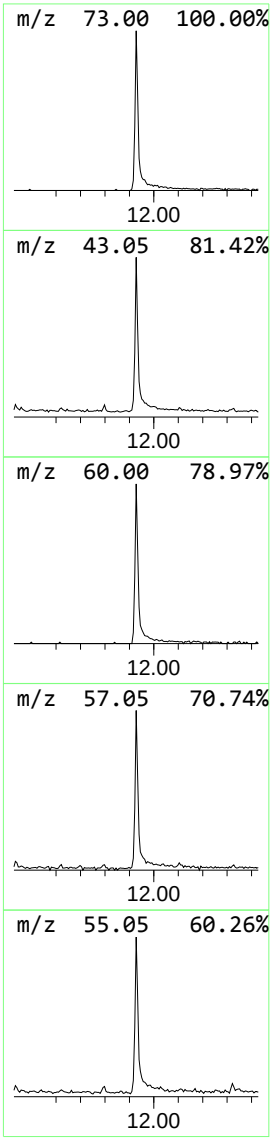
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	5.17 ng	531662	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35





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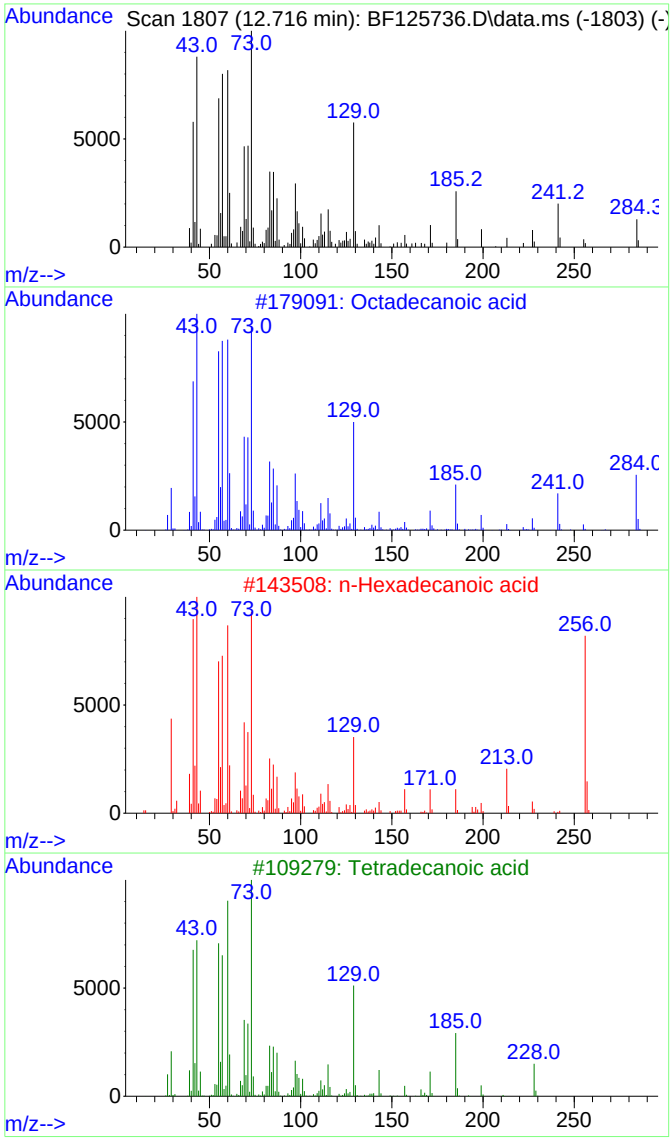
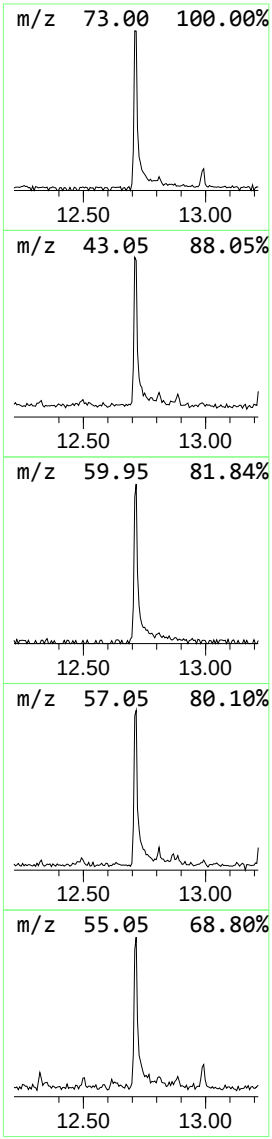
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.47 ng	254047	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





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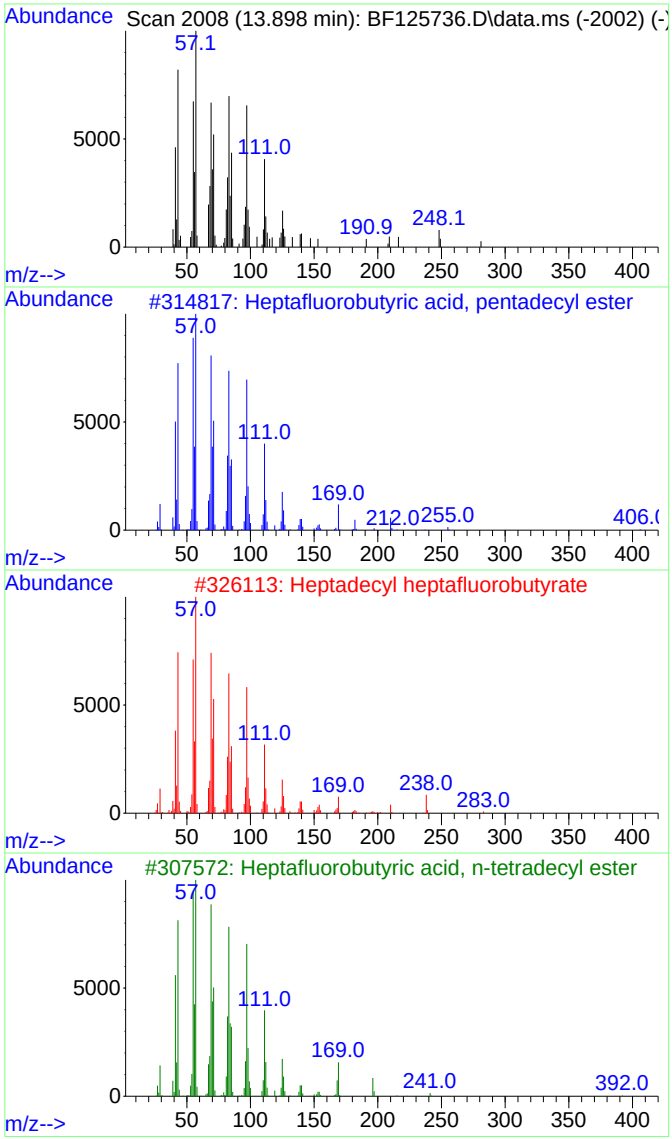
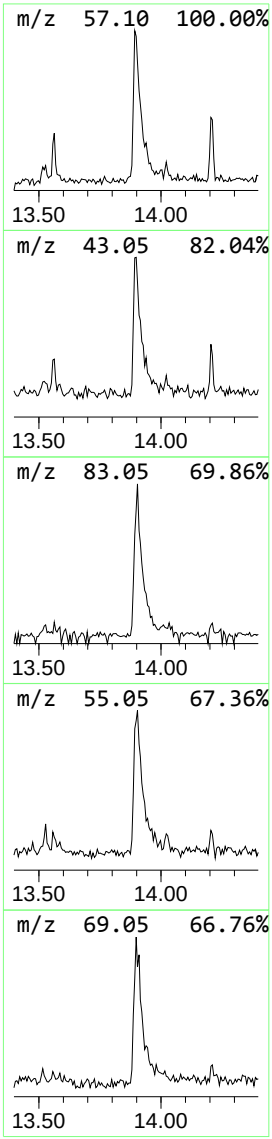
Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.95 ng	224305	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.187	83.9	ng	5045760	1	6.887	1203200	20.0
Benzothiazole, ...	8.857	4.0	ng	337854	2	8.169	1673960	20.0
n-Hexadecanoic ...	11.928	5.2	ng	531662	4	11.404	2056770	20.0
Octadecanoic acid	12.716	2.5	ng	254047	4	11.404	2056770	20.0
Heptafluorobuty...	13.898	3.0	ng	224305	5	14.039	1520190	20.0