LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136104.D
Acq On : 02 Nov 2023 19:32
Operator : CG\JU
Sample : 05049-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4

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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	508	rVB	68800	77506	1.97%	0.406%
2	5.446	566	571	574	rBV	1583591	1431435	36.44%	7.500%
3	6.445	737	741	744	rBV	1113820	911093	23.19%	4.774%
4	6.816	801	804	808	rBV	894997	702470	17.88%	3.680%
5	6.881	811	815	825	rBV	57711	71691	1.82%	0.376%
6	7.387	895	901	903	rBV	2286917	2233863	56.86%	11.704%
7	7.457	910	913	918	rBV2	66141	65982	1.68%	0.346%
8	8.004	1003	1006	1010	rBV	54340	55017	1.40%	0.288%
9	8.098	1018	1022	1025	rBV	1246361	929063	23.65%	4.868%
10	8.445	1075	1081	1085	rBV	108981	115755	2.95%	0.606%
11	9.181	1202	1206	1209	rBV	4435594	3928573	100.00%	20.583%
12	9.857	1317	1321	1324	rBV	1273239	993647	25.29%	5.206%
13	10.269	1388	1391	1395	rVB	151553	115426	2.94%	0.605%
14	10.651	1451	1456	1459	rBV	2227485	2031011	51.70%	10.641%
15	11.345	1571	1574	1578	rVB	961446	863391	21.98%	4.524%
16	11.886	1662	1666	1670	rBV	72371	74039	1.88%	0.388%
17	12.769	1812	1816	1822	rBV	243925	197746	5.03%	1.036%
18	12.951	1842	1847	1850	rBV	3298621	2966242	75.50%	15.541%
19	12.980	1850	1852	1858	rVB	167517	129358	3.29%	0.678%
20	13.886	1999	2006	2019	rBV10	19161	72075	1.83%	0.378%
21	14.004	2022	2026	2030	rVB	693617	605372	15.41%	3.172%
22	15.492	2274	2279	2285	rBV	431109	515571	13.12%	2.701%

Sum of corrected areas: 19086326

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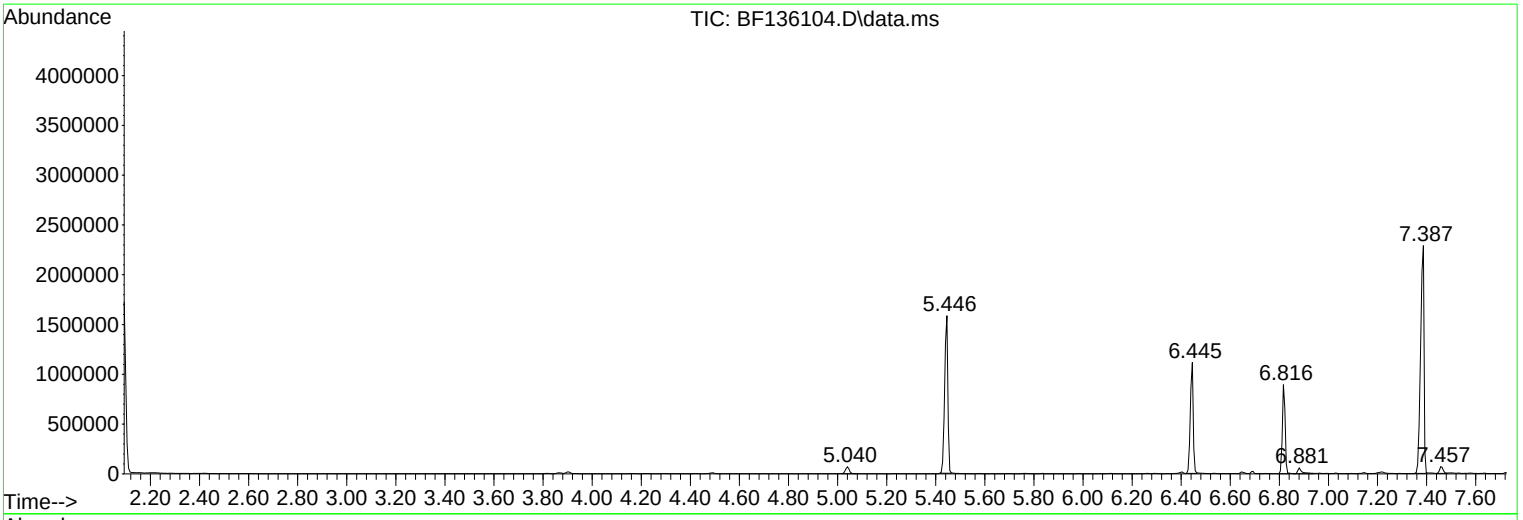
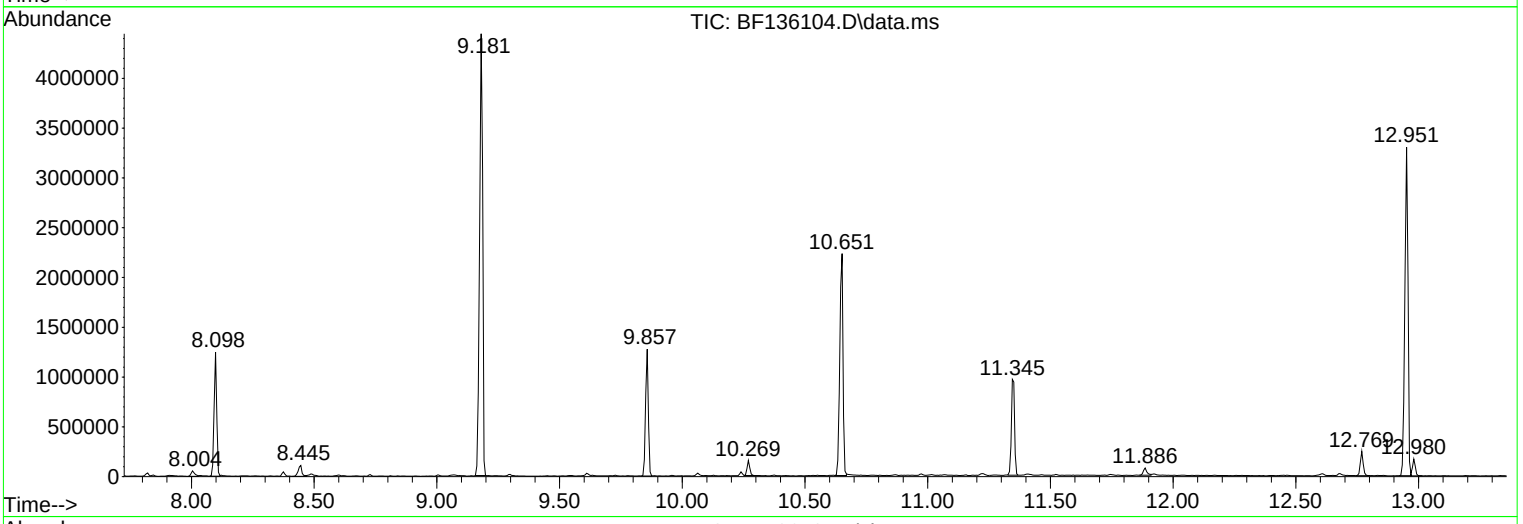
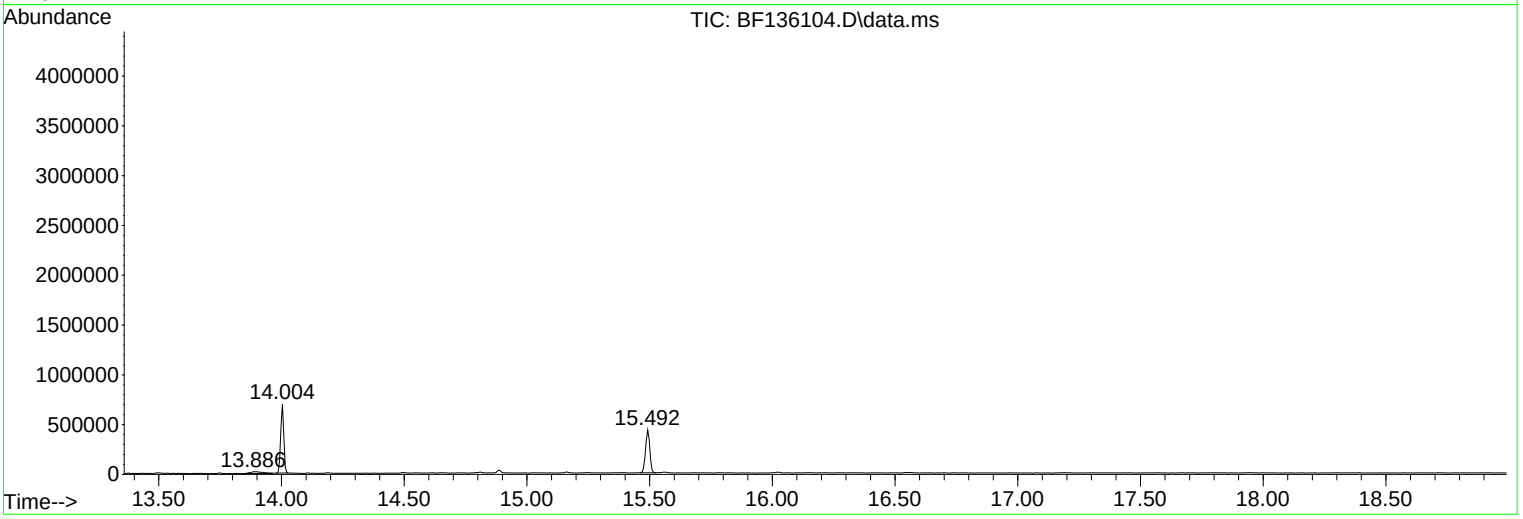
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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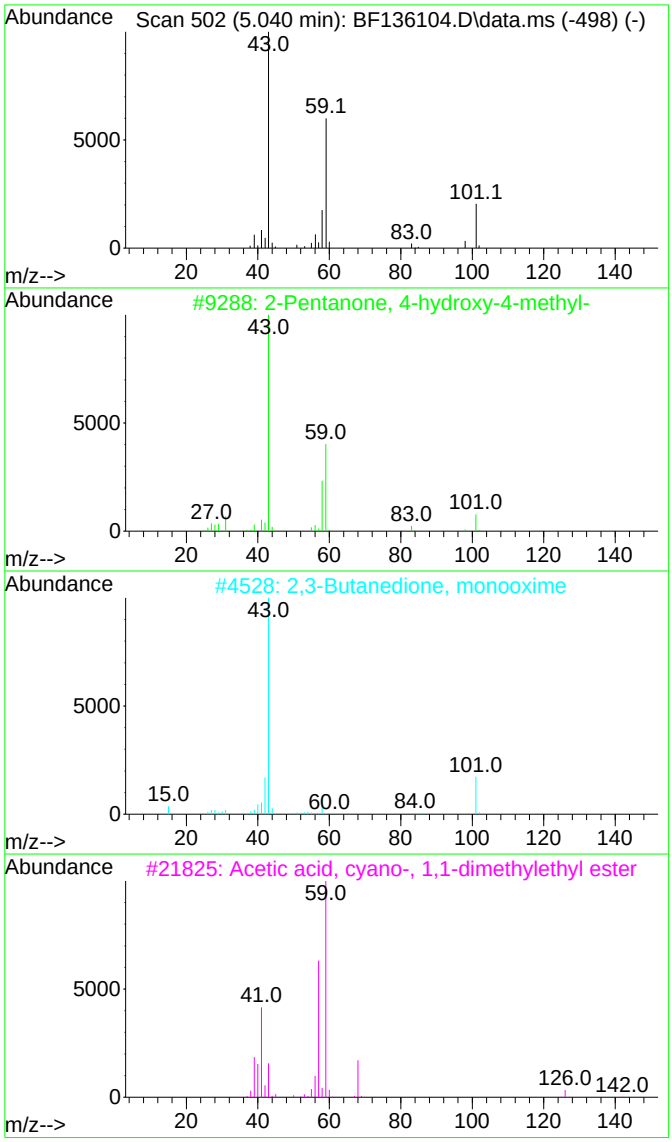
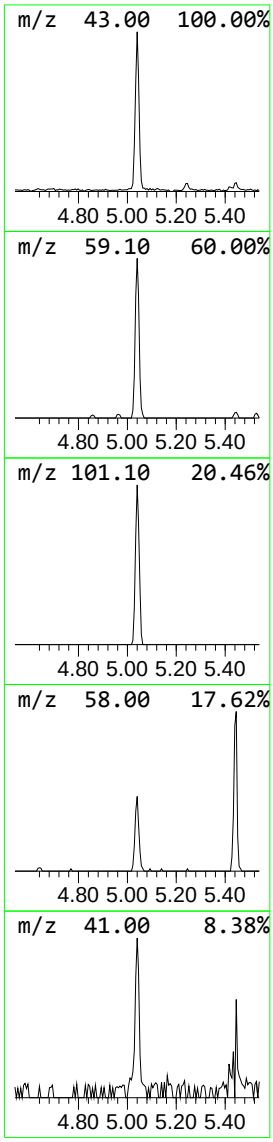
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.21 ng	77506	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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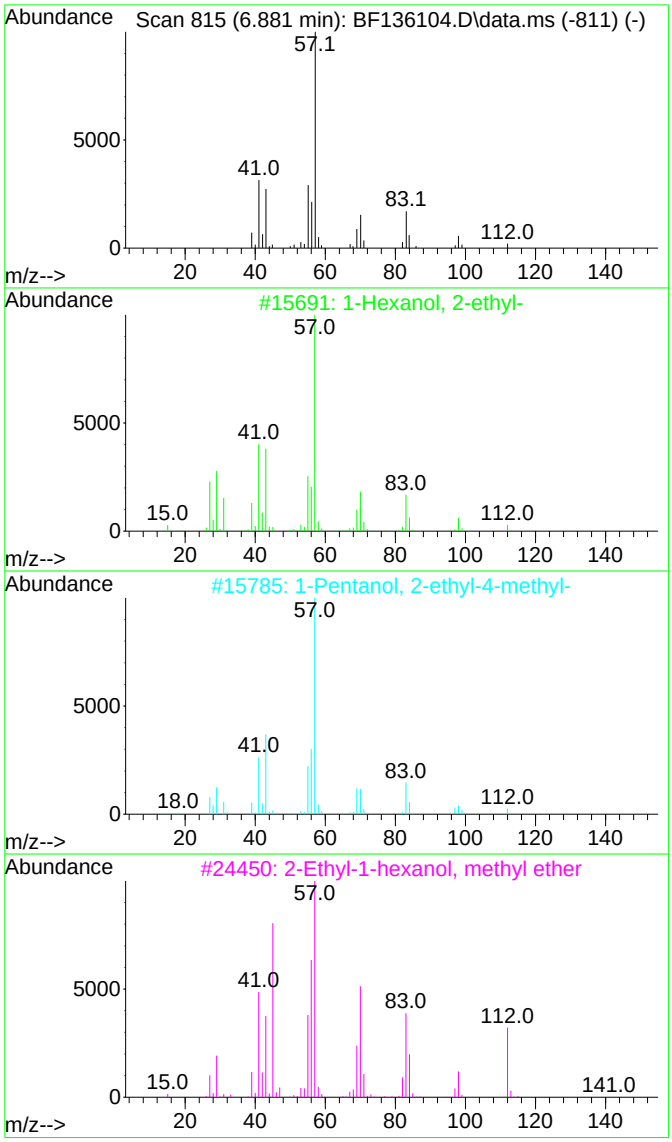
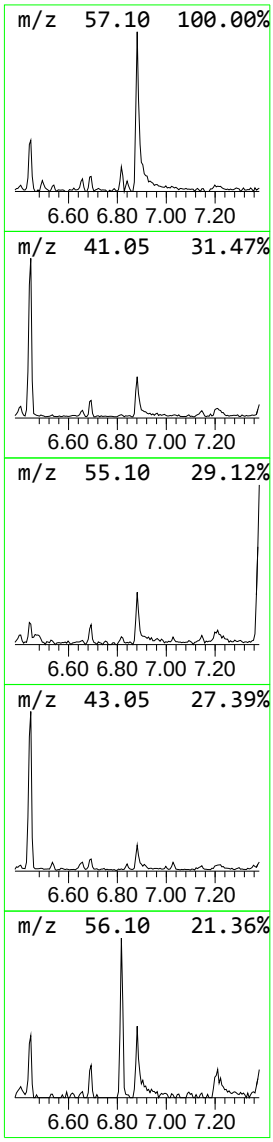
****
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.881	2.04 ng	71691	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	78
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	59
4	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	53
5	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	47





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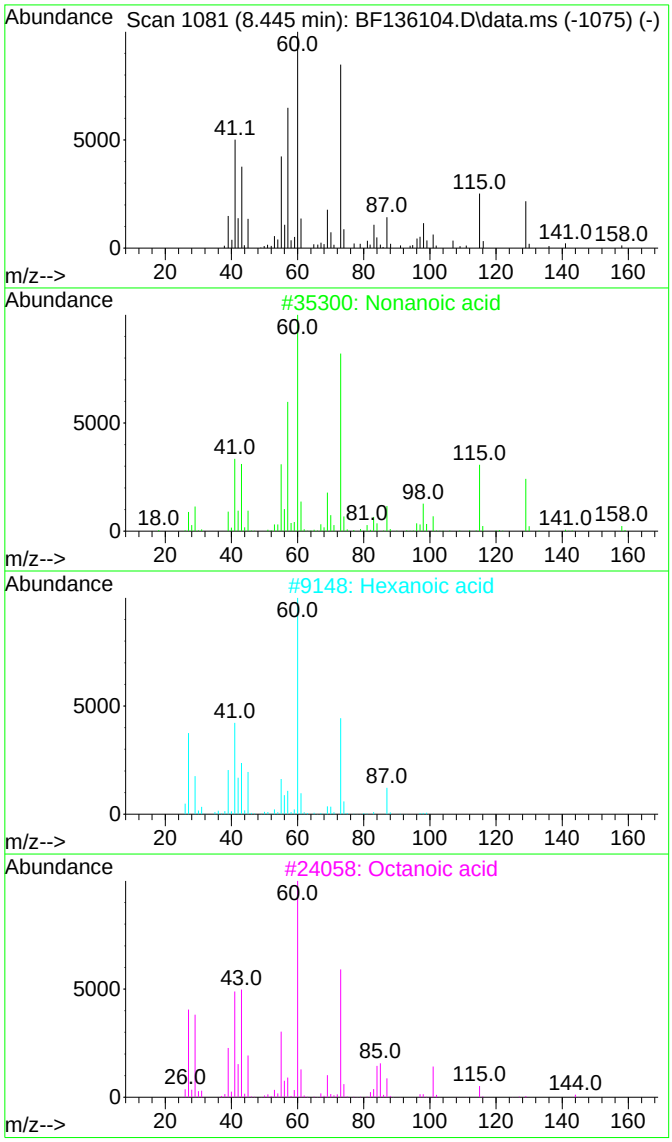
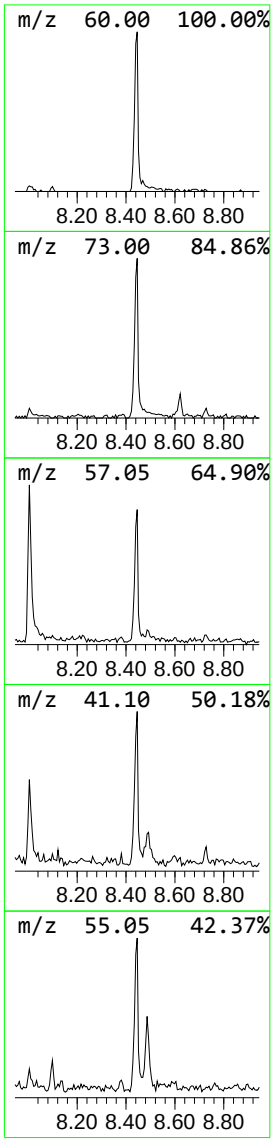
****

Peak Number 3 Nonanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	2.49 ng	115755	Naphthalene-d8	8.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	95
2	Hexanoic acid	116	C6H12O2	000142-62-1	50
3	Octanoic acid	144	C8H16O2	000124-07-2	50
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43





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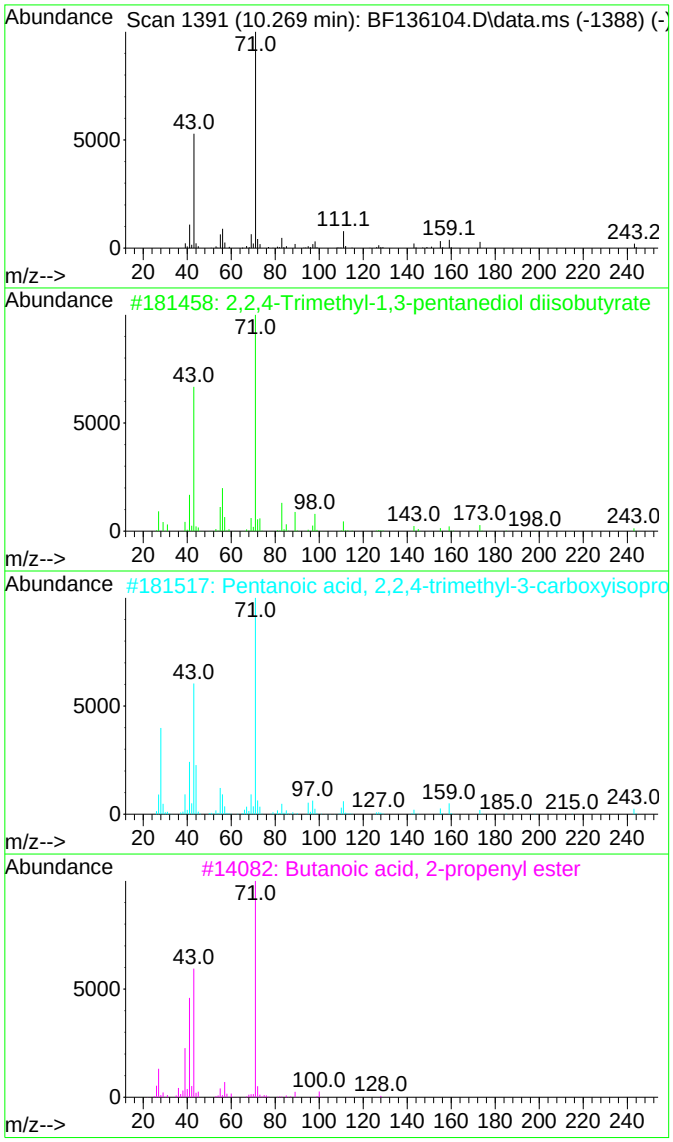
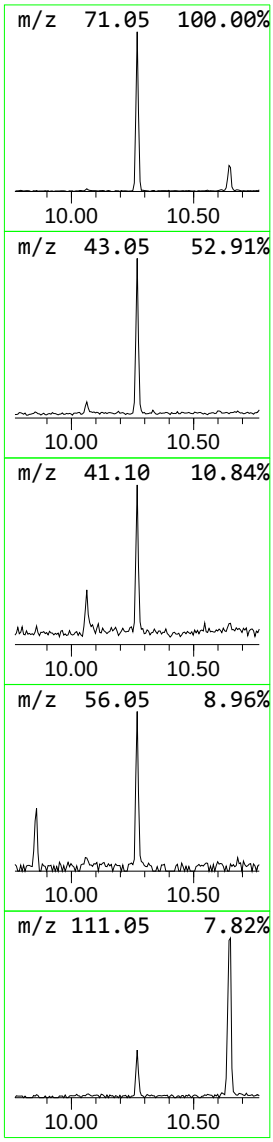
****
Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.269	2.32 ng	115426	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78
2	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	64
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	59
4	Propanoic acid, 2-methyl-, 1,2,3...	302	C15H26O6	014295-64-8	50
5	(2R,3R)-2,3-Dihydroxybutanedioic...	248	C10H16O7	1000462-99-8	50





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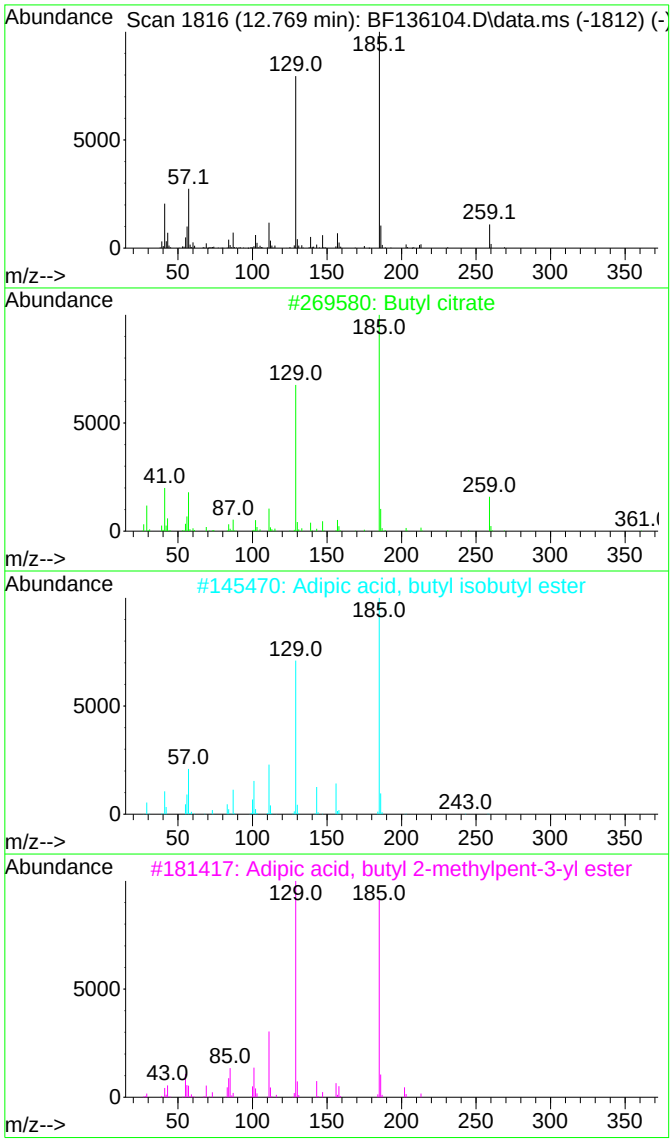
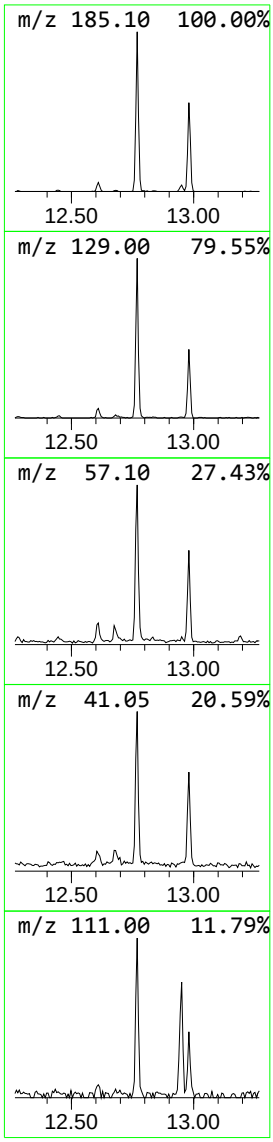
****

Peak Number 5 Butyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.769	6.53 ng	197746	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	81
2	Adipic acid, butyl isobutyl ester	258	C14H26O4	1010324-09-3	64
3	Adipic acid, butyl 2-methylpent-...	286	C16H30O4	1010353-55-8	56
4	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	56
5	Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	56





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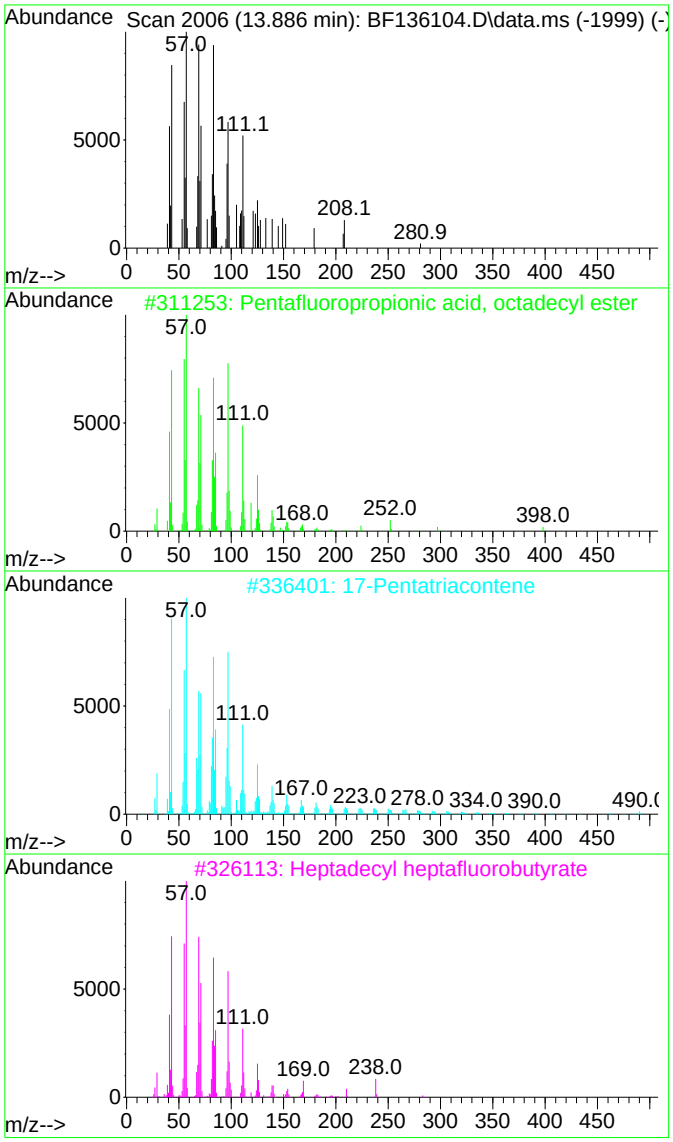
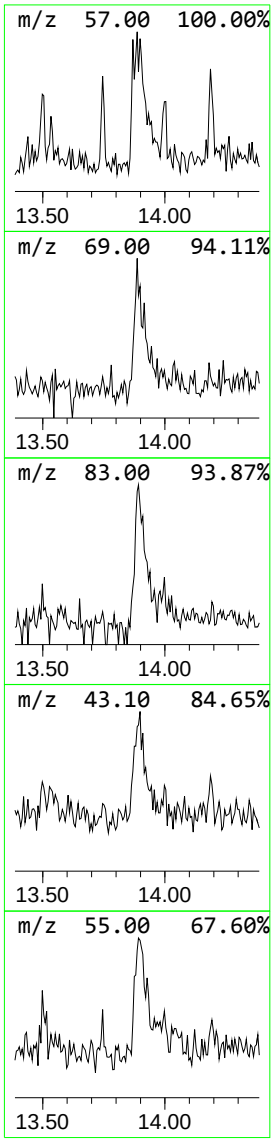
****
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.38 ng	72075	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	55
2	17-Pentatriacontene	491	C35H70	006971-40-0	53
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	52
4	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	49
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	49





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-...	5.040	2.2	ng	77506	1	6.816	702470	20.0
1-Hexanol, 2-et...	6.881	2.0	ng	71691	1	6.816	702470	20.0
Nonanoic acid	8.445	2.5	ng	115755	2	8.098	929063	20.0
2,2,4-Trimethyl...	10.269	2.3	ng	115426	3	9.857	993647	20.0
Butyl citrate	12.769	6.5	ng	197746	5	14.004	605372	20.0
Pentafluoroprop...	13.886	2.4	ng	72075	5	14.004	605372	20.0