LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139854.D
Acq On : 18 Oct 2024 15:21
Operator : RC/JU
Sample : P4405-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-121

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	5	14	21	rVB	5326392	9085089	100.00%	25.533%
2	5.104	505	512	519	rVB	101421	154976	1.71%	0.436%
3	5.498	573	579	584	rBV	2136515	2776449	30.56%	7.803%
4	6.498	743	749	754	rBV	1671744	2156151	23.73%	6.060%
5	6.887	810	815	820	rBV	768239	943948	10.39%	2.653%
6	7.445	904	910	916	rBV	2208010	3046133	33.53%	8.561%
7	8.169	1028	1033	1038	rBV	973196	1189887	13.10%	3.344%
8	9.245	1210	1216	1221	rBV	3901381	4952395	54.51%	13.918%
9	9.922	1326	1331	1336	rBV	990694	1213819	13.36%	3.411%
10	10.633	1447	1452	1459	rVB	148476	189885	2.09%	0.534%
11	10.710	1459	1465	1470	rBV	2014913	2576531	28.36%	7.241%
12	11.410	1579	1584	1589	rBV	813256	1002774	11.04%	2.818%
13	11.933	1667	1673	1695	rBV2	178345	371979	4.09%	1.045%
14	12.716	1801	1806	1818	rBV	86048	155915	1.72%	0.438%
15	12.998	1848	1854	1859	rBV	2946744	3841962	42.29%	10.797%
16	13.904	2002	2008	2021	rBV	66677	134610	1.48%	0.378%
17	14.045	2025	2032	2040	rVB	761222	1029061	11.33%	2.892%
18	15.521	2277	2283	2288	rBV	499729	760670	8.37%	2.138%

Sum of corrected areas: 35582234

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ClientSampleId :
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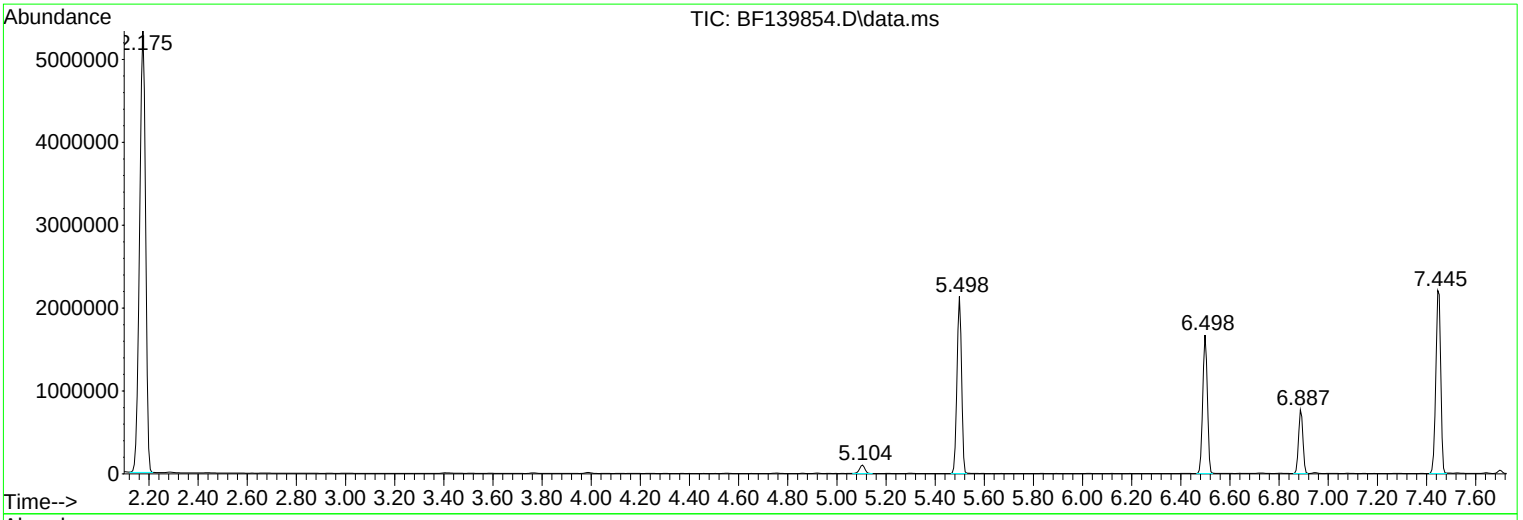
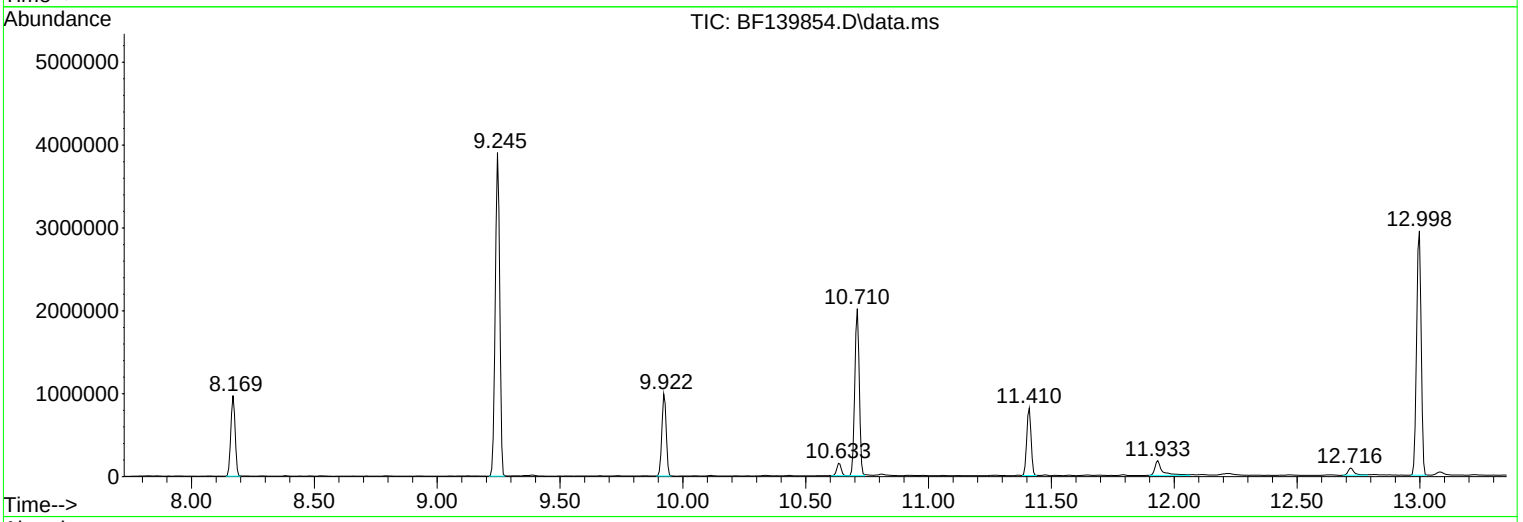
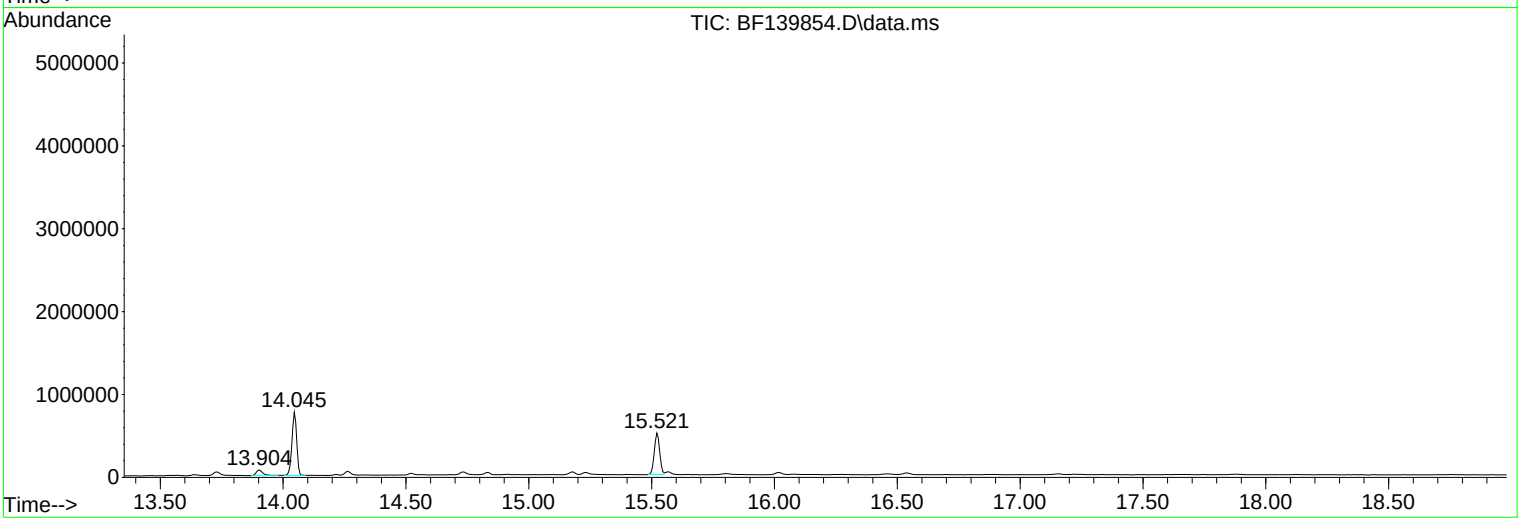
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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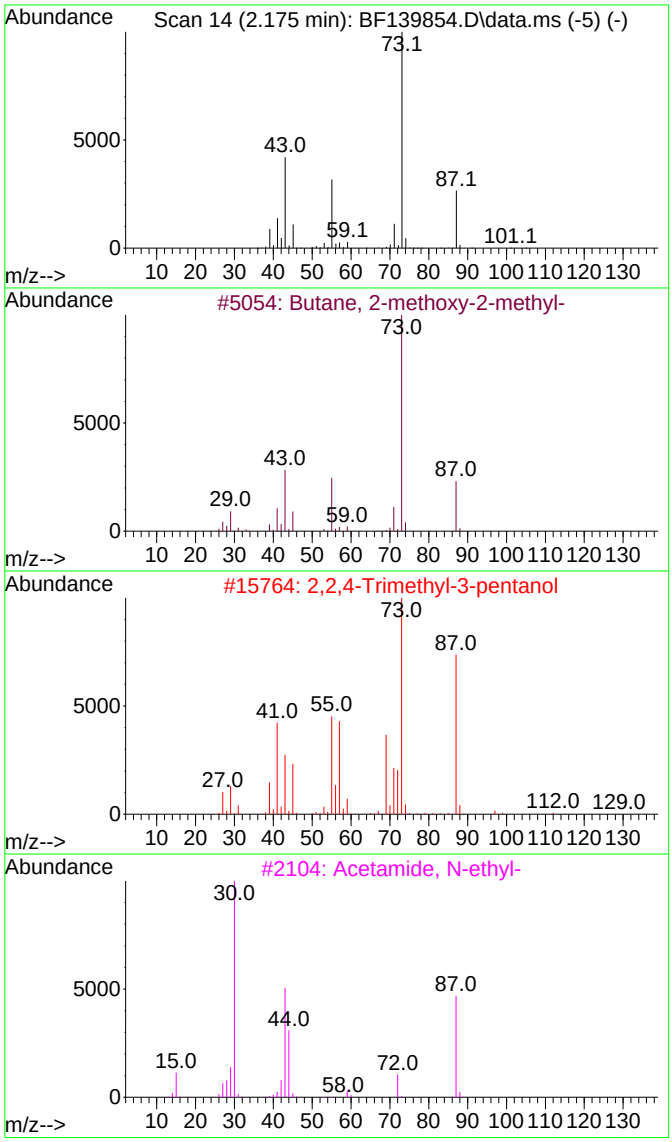
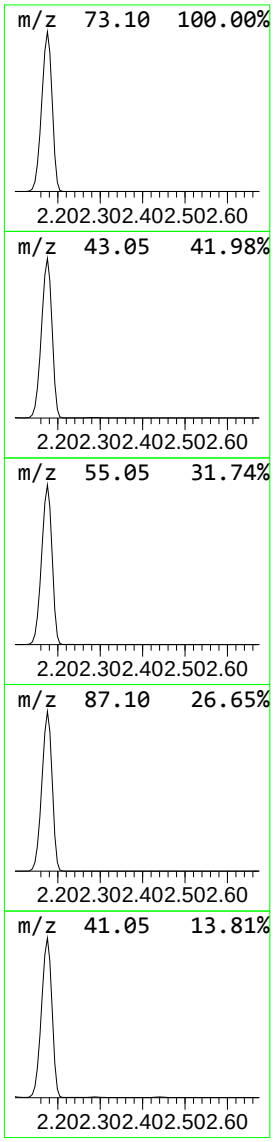
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	192.49 ng	9085090	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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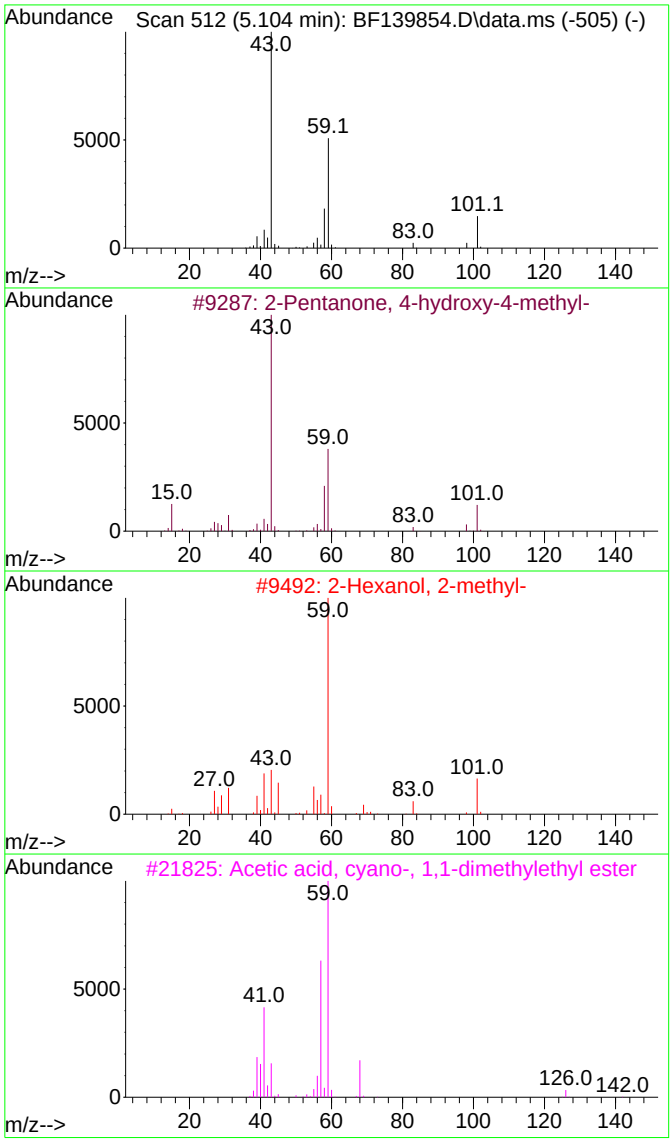
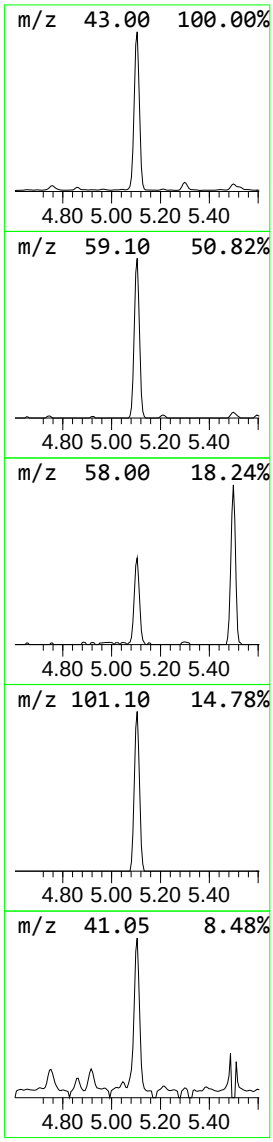
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.28 ng	154976	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Operator : RC/JU
Sample : P4405-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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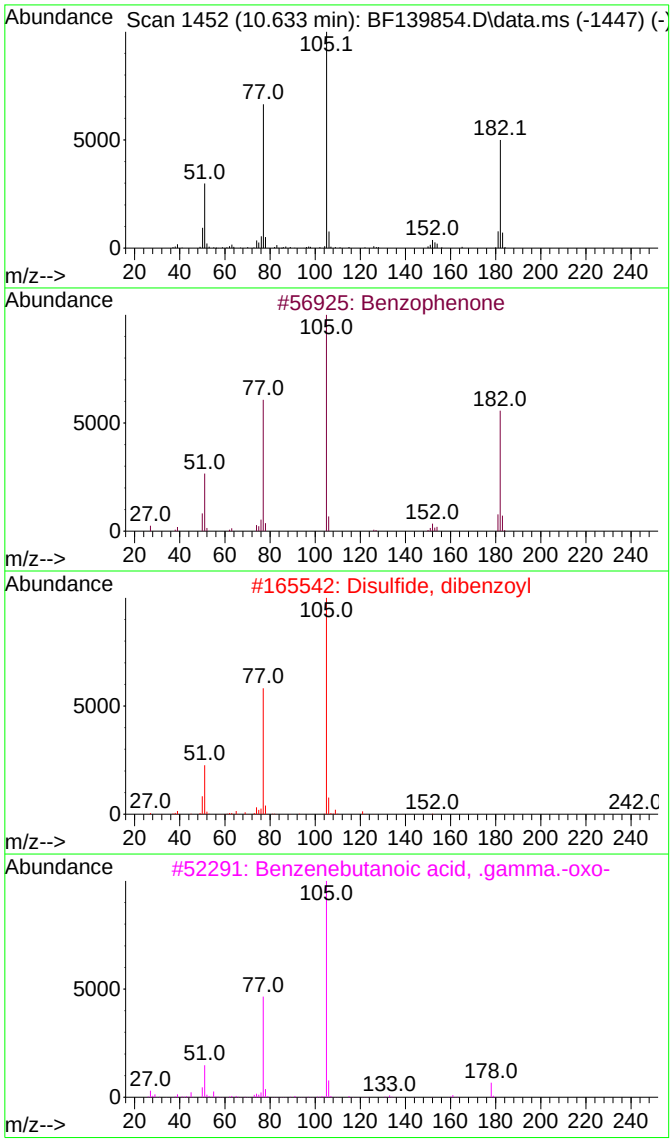
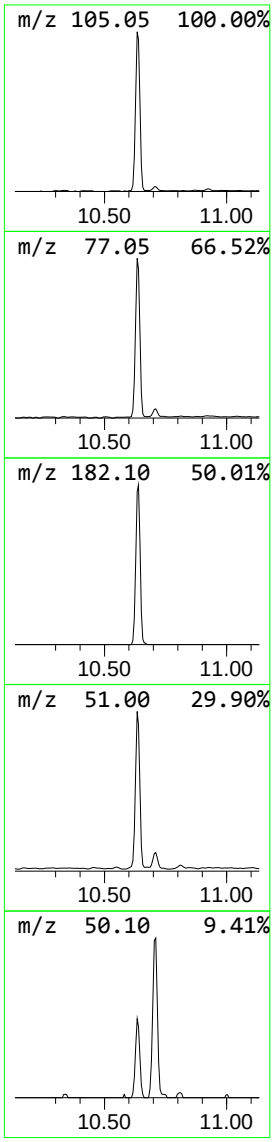
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	3.13 ng	189885	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	50
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
5	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50





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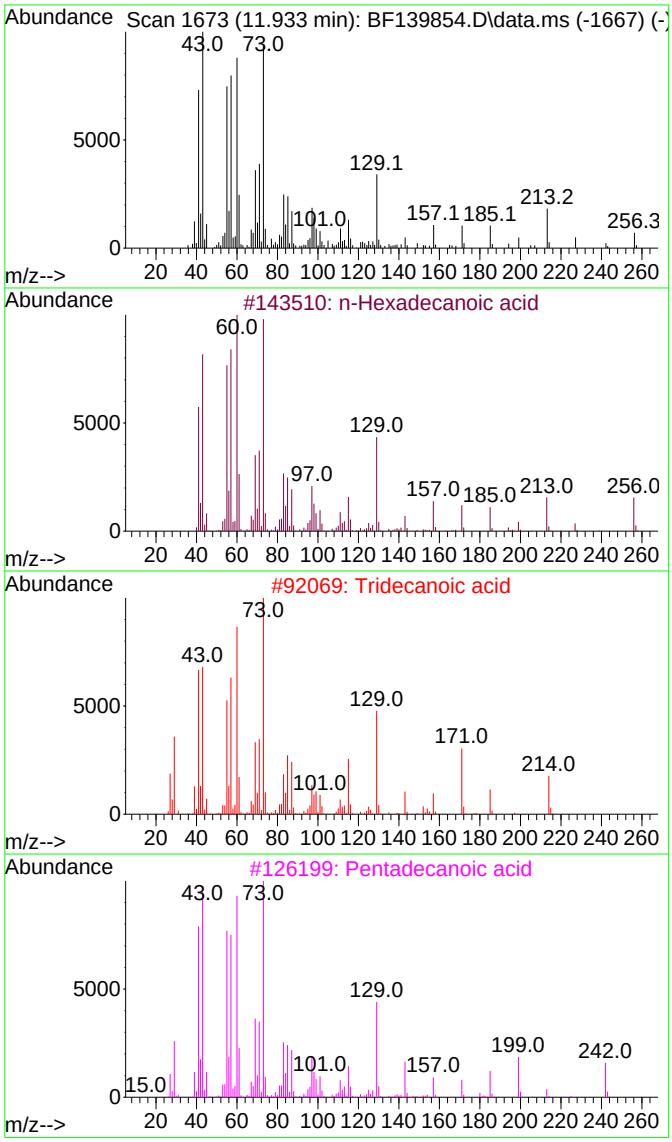
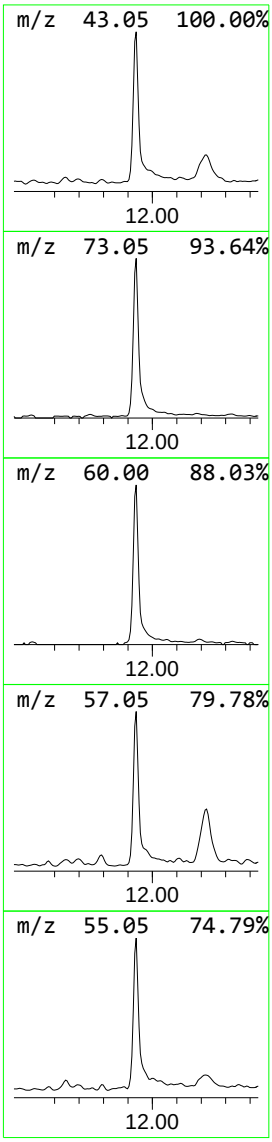
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.42 ng	371979	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octanoic acid	144	C8H16O2	000124-07-2	49





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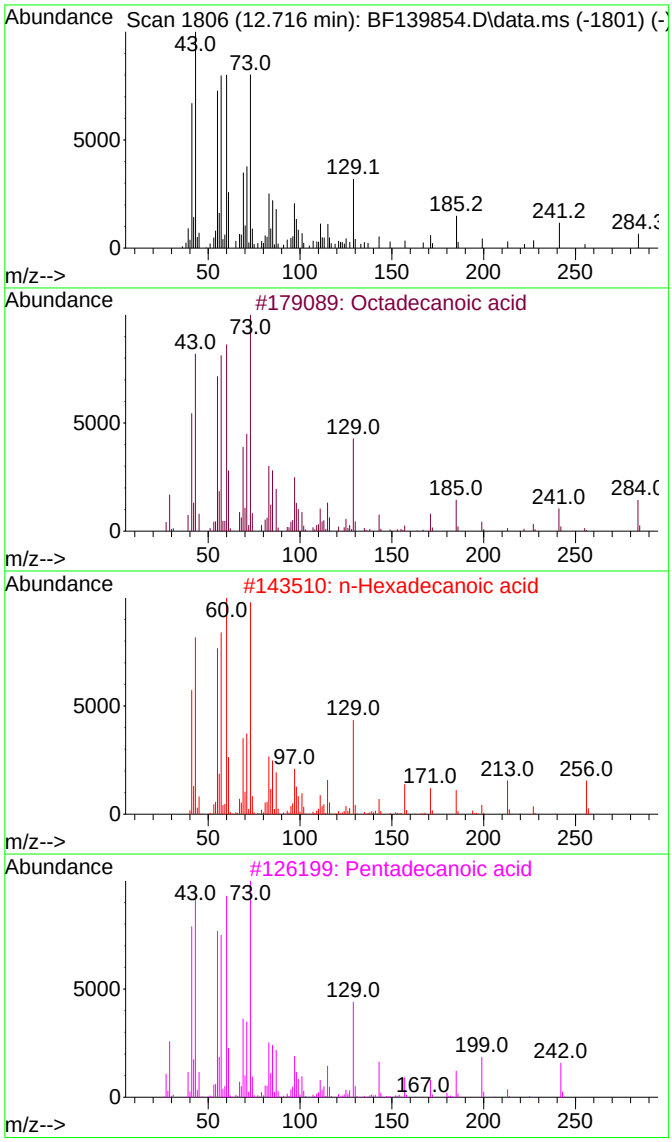
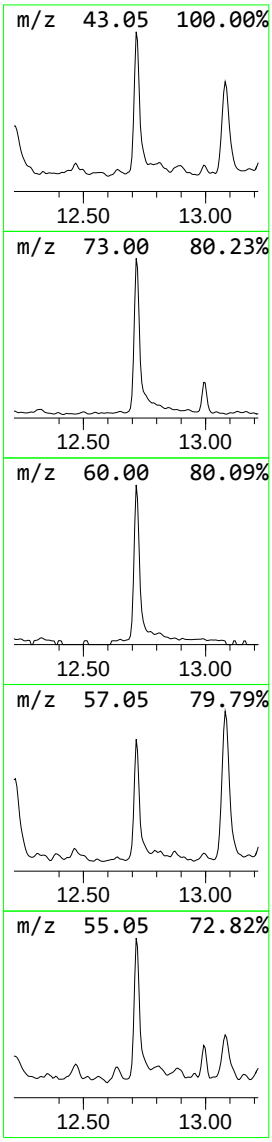
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.11 ng	155915	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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TIC Library : C:\Database\NIST20.L
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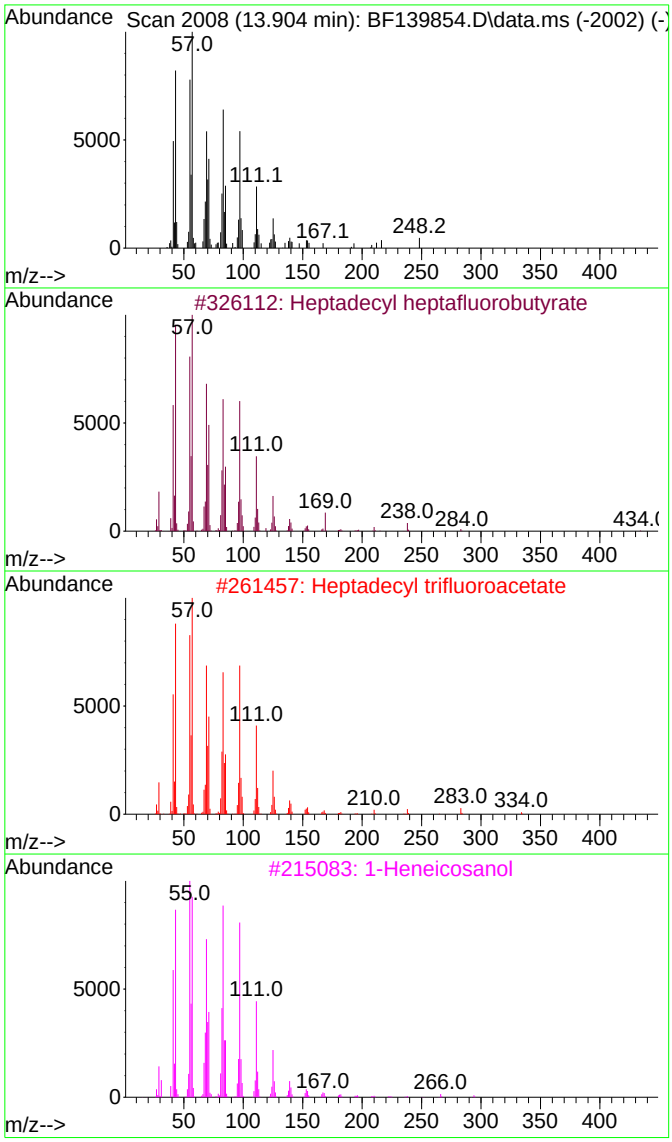
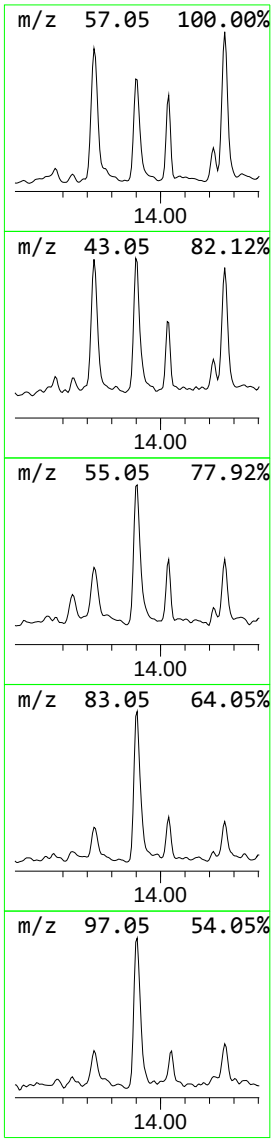
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.62 ng	134610	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.175	192.5	ng	9085090	1	6.887	943948	20.0
2-Pentanone, 4-...	5.104	3.3	ng	154976	1	6.887	943948	20.0
Benzophenone	10.633	3.1	ng	189885	3	9.922	1213820	20.0
n-Hexadecanoic ...	11.933	7.4	ng	371979	4	11.410	1002770	20.0
Octadecanoic acid	12.716	3.1	ng	155915	4	11.410	1002770	20.0
Heptadecyl hept...	13.904	2.6	ng	134610	5	14.045	1029060	20.0