LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
Data File : BF132170.D
Acq On : 20 Jan 2023 20:03
Operator : CG\JU
Sample : 01233-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P34A

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-BF011923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.343	420	426	438	rVB	1595638	2340160	37.75%	5.482%
2	5.719	484	490	493	rBV	4359832	5094324	82.17%	11.934%
3	6.701	651	657	660	rBV	4059404	5288414	85.30%	12.389%
4	7.090	719	723	726	rBV	1245877	992766	16.01%	2.326%
5	7.654	813	819	822	rBV	3606612	3467630	55.93%	8.123%
6	8.378	938	942	945	rBV	1410037	1268443	20.46%	2.971%
7	9.454	1119	1125	1128	rBV	6135162	5566542	89.79%	13.040%
8	10.142	1238	1242	1245	rBV	1726414	1459040	23.53%	3.418%
9	10.860	1360	1364	1367	rBV	1687039	1478355	23.85%	3.463%
10	10.936	1372	1377	1380	rBV	4620949	4354265	70.23%	10.200%
11	11.166	1412	1416	1422	rBV	256198	201384	3.25%	0.472%
12	11.636	1493	1496	1500	rBV	1762152	1570274	25.33%	3.679%
13	12.148	1575	1583	1588	rBV	469968	436622	7.04%	1.023%
14	12.936	1713	1717	1723	rBV	121218	118092	1.90%	0.277%
15	13.236	1763	1768	1771	rBV	6294525	6199653	100.00%	14.523%
16	14.124	1916	1919	1945	rBV3	158024	501868	8.10%	1.176%
17	14.301	1945	1949	1953	rBV	1462189	1308482	21.11%	3.065%
18	15.895	2214	2220	2232	rBV2	742312	1041172	16.79%	2.439%

Sum of corrected areas: 42687486

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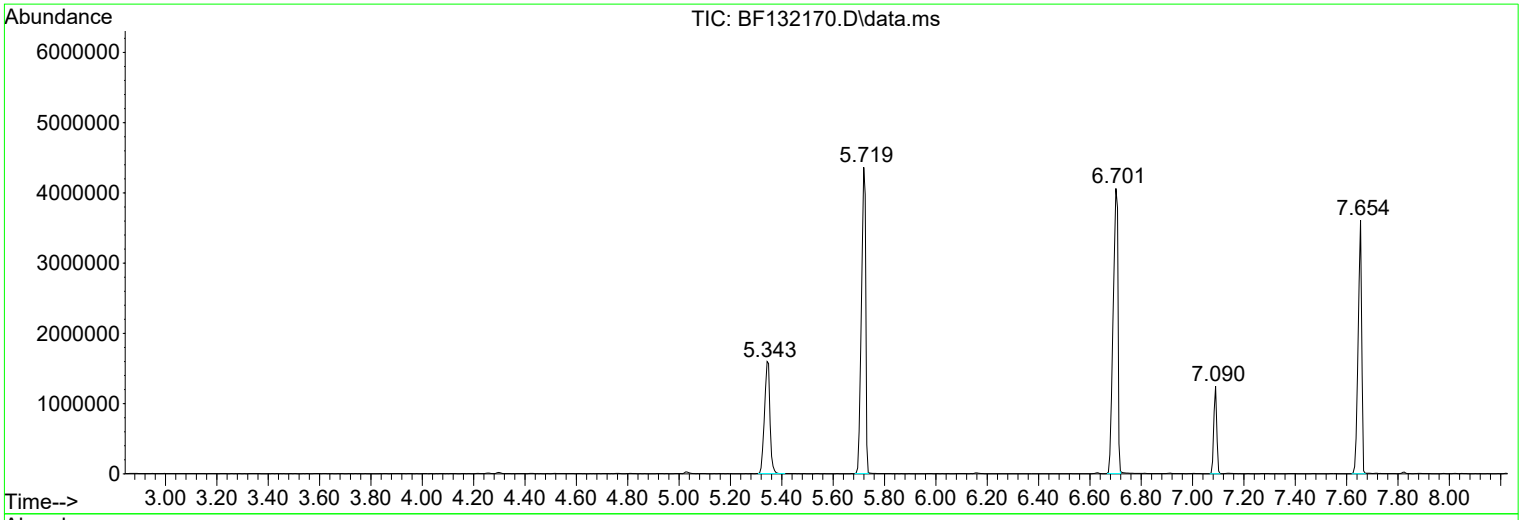
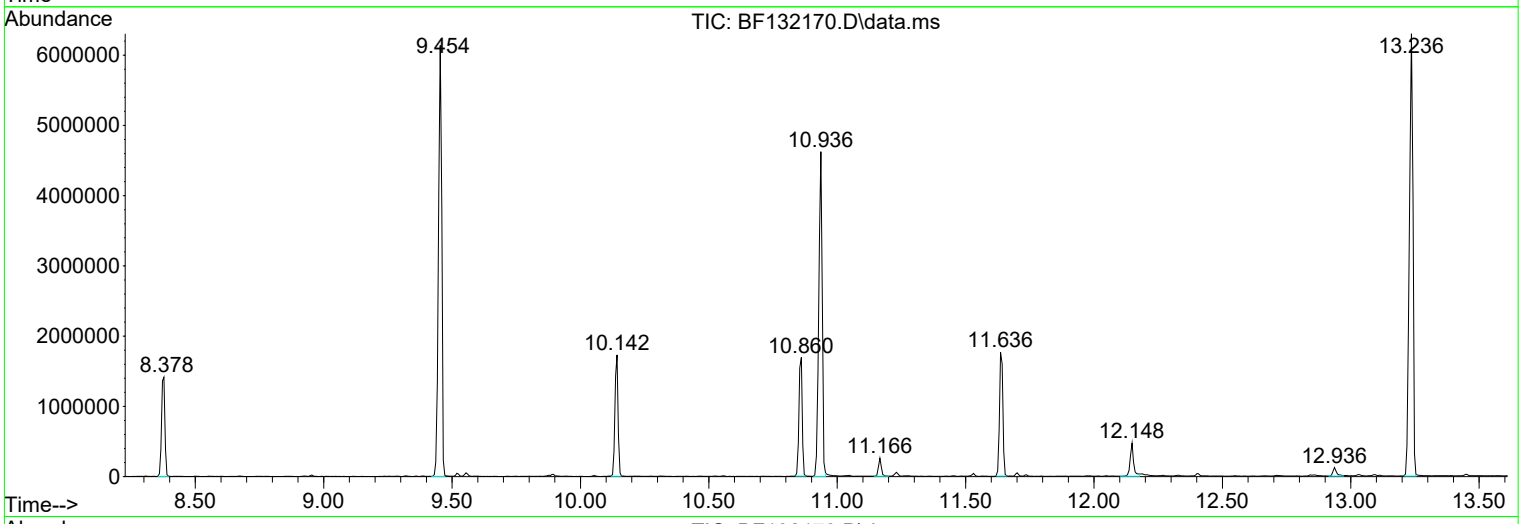
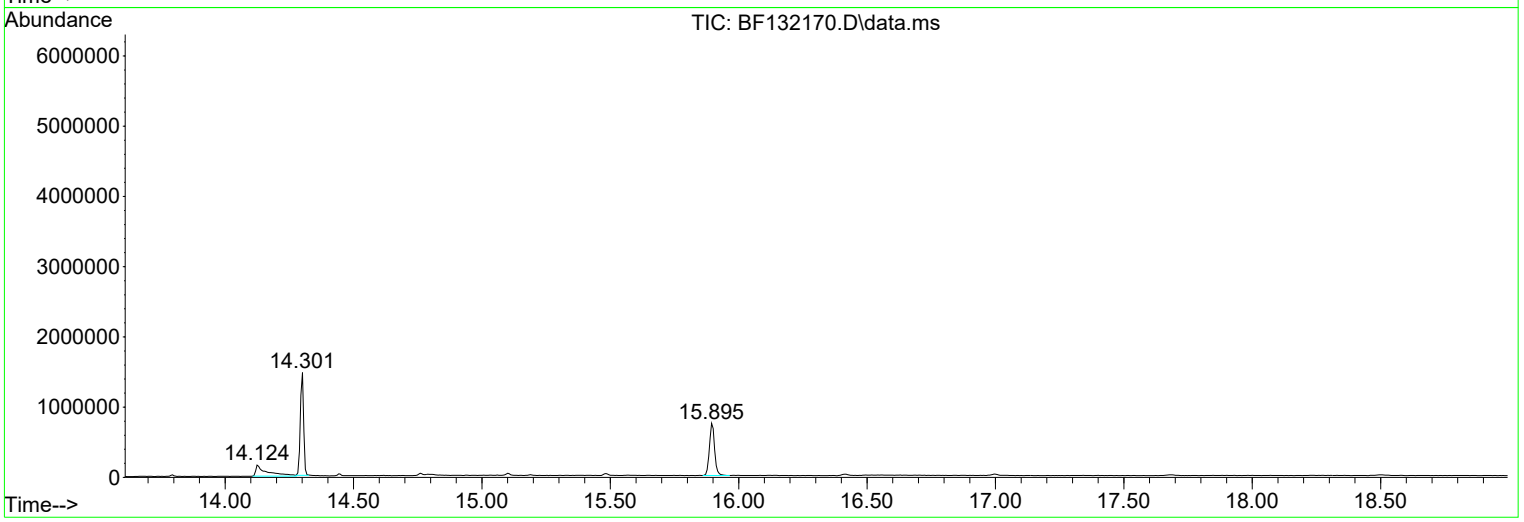
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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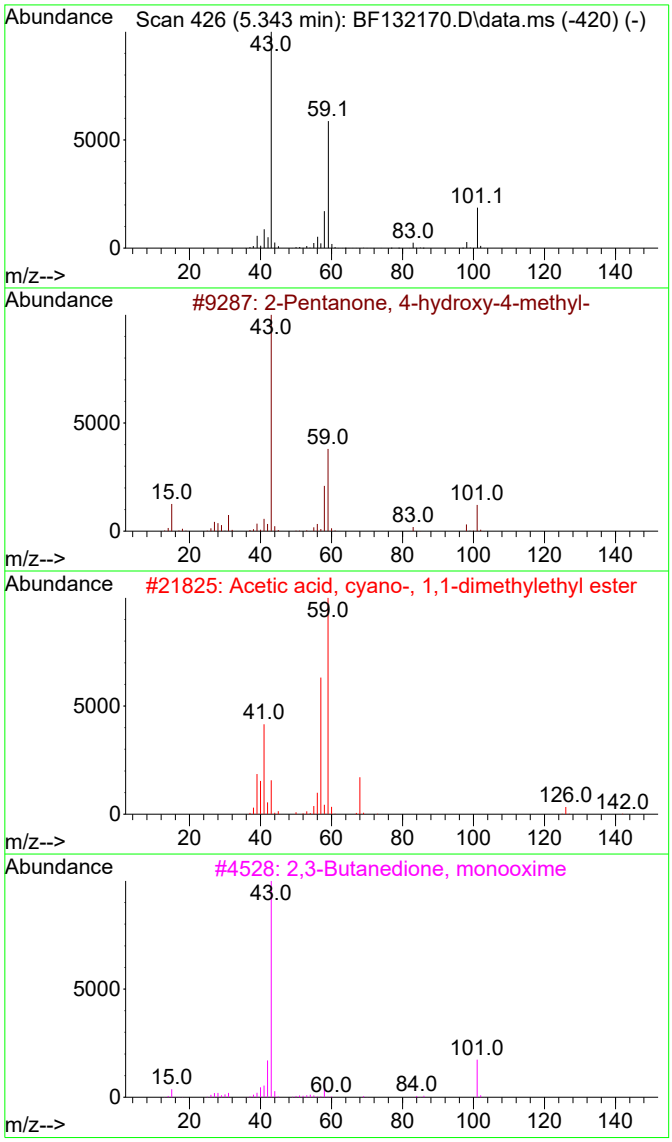
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

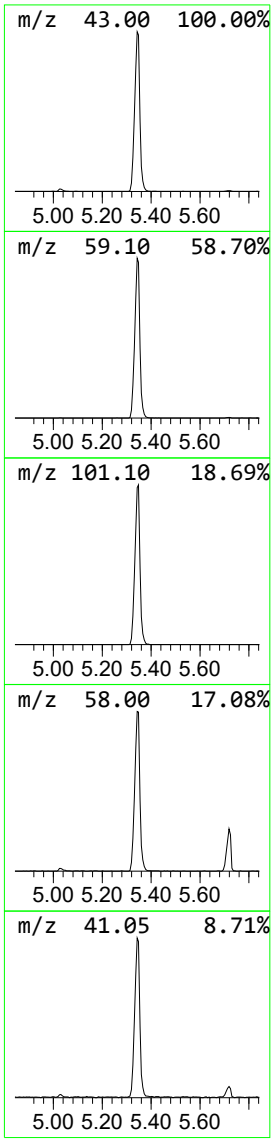
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.343	47.14 ng	2340160	1,4-Dichlorobenzene-d4	7.090

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Acetone	58	C3H6O	000067-64-1	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

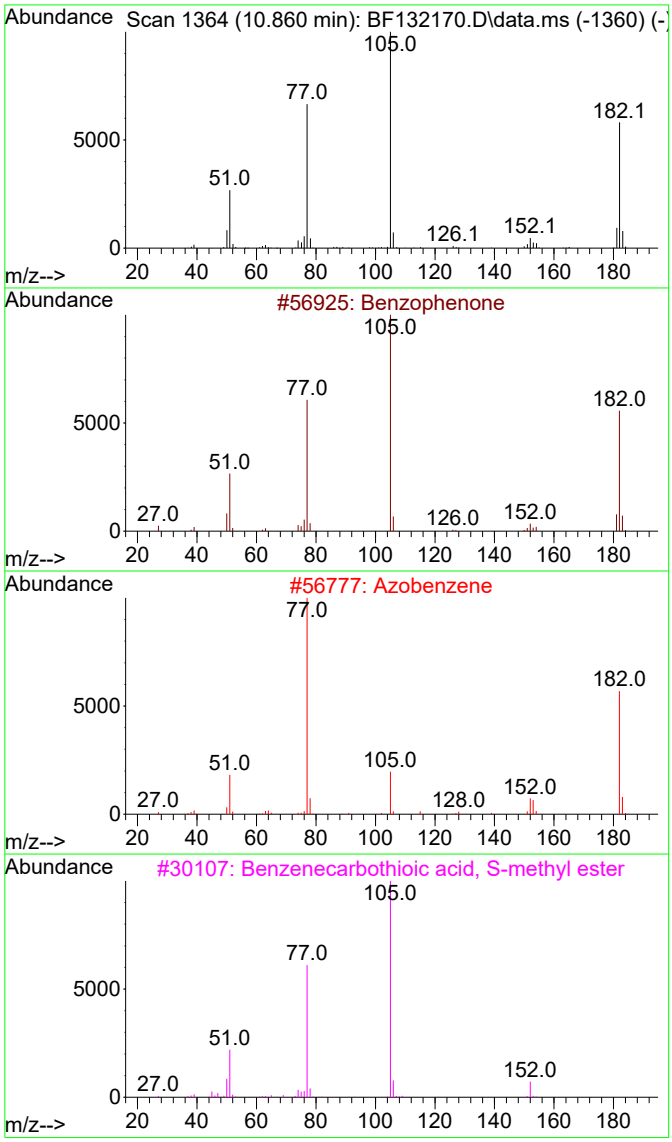
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

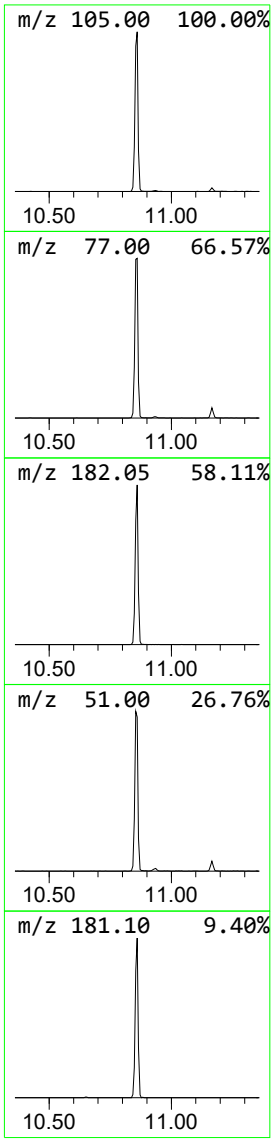
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	20.26 ng	1478360	Acenaphthene-d10	10.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47





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Instrument :
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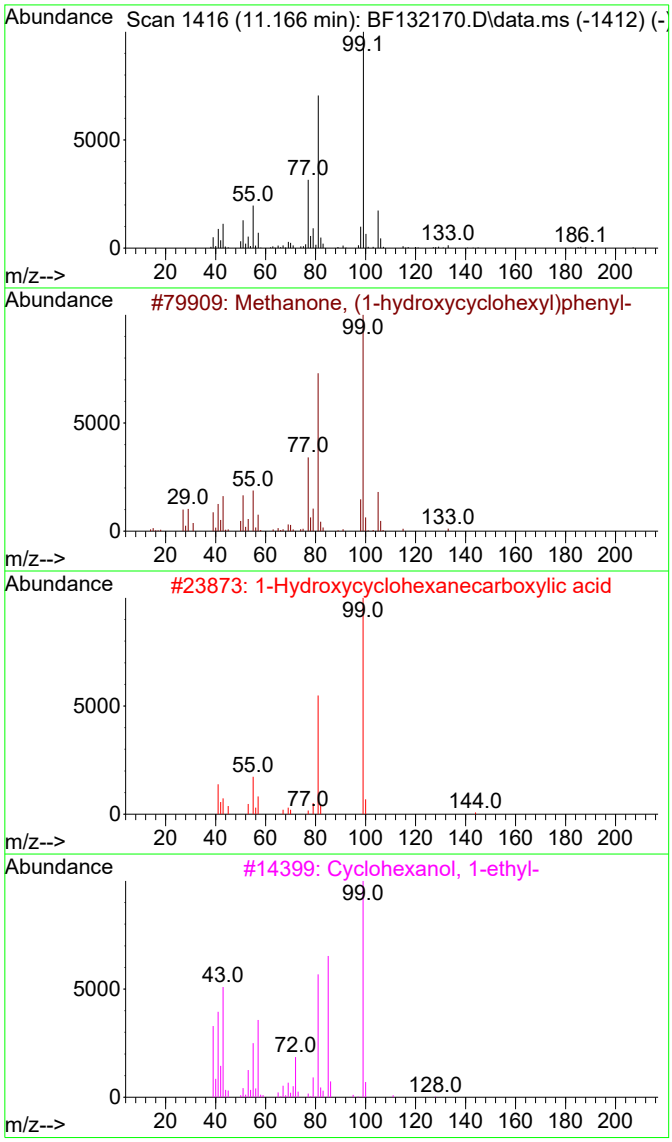
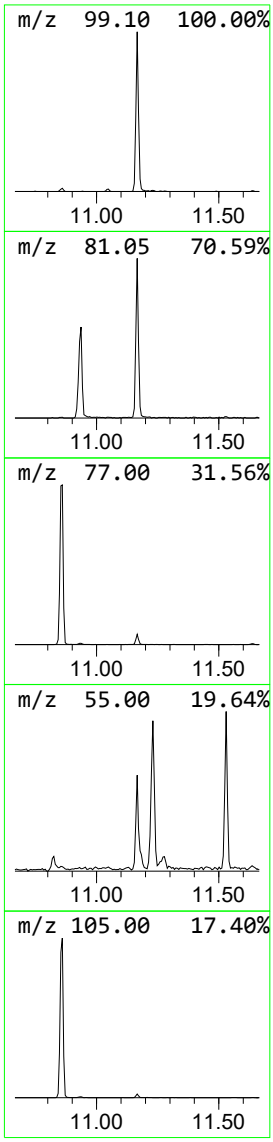
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methanone, (1-hydroxycycloh... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.166	2.56 ng	201384	Phenanthrene-d10	11.636

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	50
3	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	50
4	1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	38
5	Hexanoic acid, thio-, S-butyl ester	188	C10H20OS	002432-79-3	38





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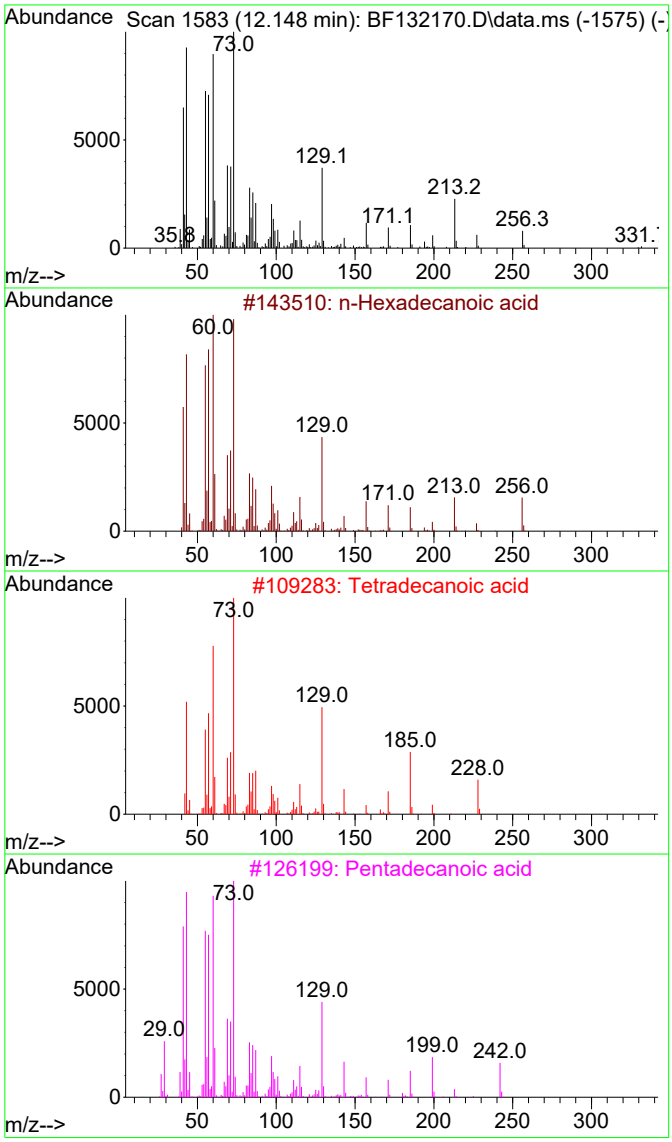
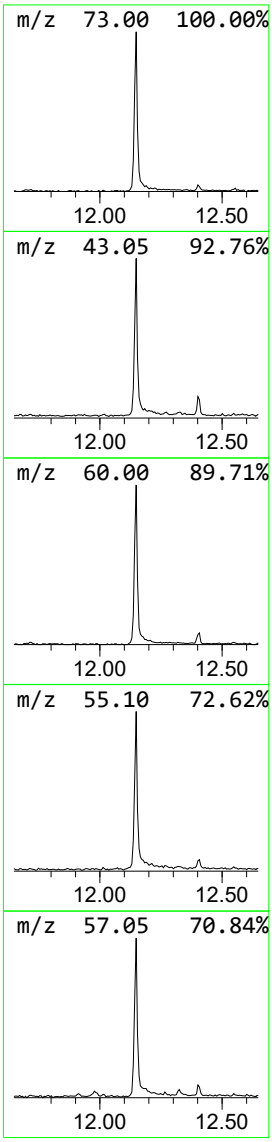
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.148	5.56 ng	436622	Phenanthrene-d10	11.636

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





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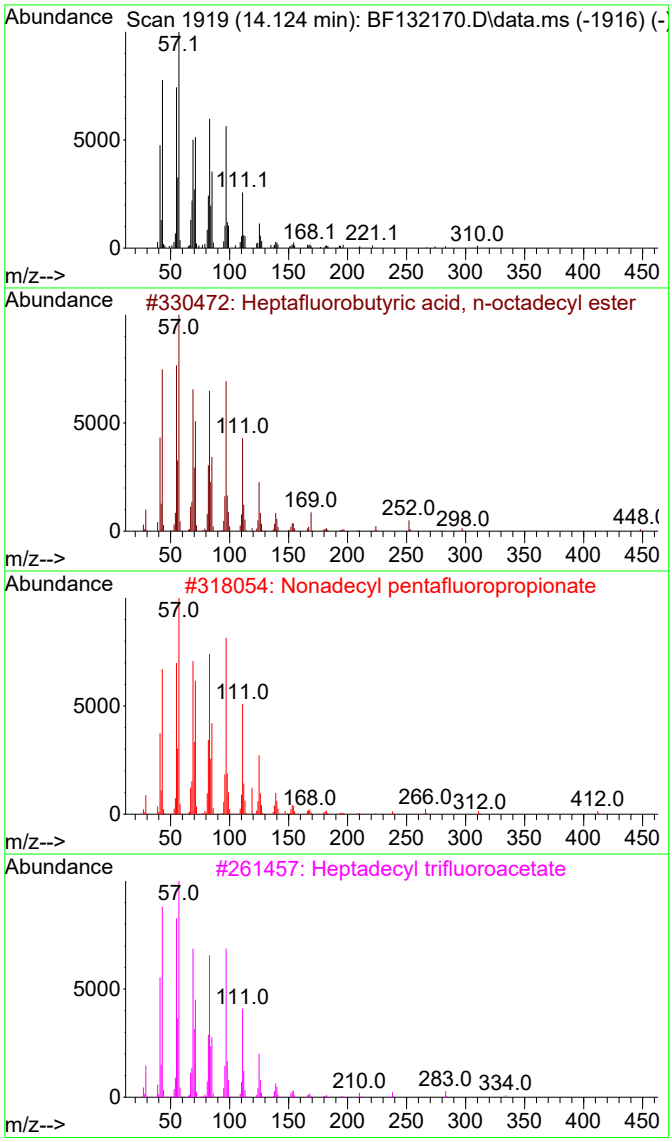
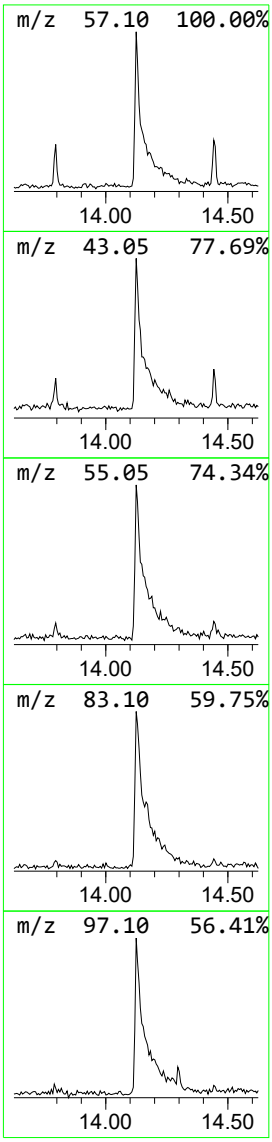
****
Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.124	7.67 ng	501868	Chrysene-d12	14.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4	Hexacosyl propyl ether	424	C29H60O	1000406-28-4	91
5	Butyl docosyl ether	382	C26H54O	1000406-40-8	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
2-Pentanone, 4-...	5.343	47.1	ng	2340160	1	7.090	992766	20.0
Benzophenone	10.860	20.3	ng	1478360	3	10.142	1459040	20.0
Methanone, (1-h...	11.166	2.6	ng	201384	4	11.636	1570270	20.0
n-Hexadecanoic ...	12.148	5.6	ng	436622	4	11.636	1570270	20.0
Heptafluorobuty...	14.124	7.7	ng	501868	5	14.301	1308480	20.0