LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133215.D
Acq On : 03 May 2023 19:19
Operator : CG\JU
Sample : 02583-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-21

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133215.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	477	482	490	rVB	178132	234857	4.99%	0.756%
2	5.340	549	553	557	rBV	3728678	3782021	80.40%	12.173%
3	6.369	723	728	731	rBV	4051109	4079092	86.72%	13.129%
4	6.728	785	789	792	rBV	1498263	1103680	23.46%	3.552%
5	7.292	880	885	888	rBV	3225251	2764913	58.78%	8.899%
6	8.010	1004	1007	1011	rBV	1897184	1509545	32.09%	4.859%
7	9.092	1186	1191	1194	rBV	5282463	4703761	100.00%	15.140%
8	9.763	1301	1305	1309	rBV	2121597	1669697	35.50%	5.374%
9	10.475	1422	1426	1429	rBV	2243407	1772905	37.69%	5.706%
10	10.551	1435	1439	1448	rBV	1284723	1119353	23.80%	3.603%
11	10.780	1475	1478	1483	rBV	262143	226729	4.82%	0.730%
12	10.875	1489	1494	1497	rBV	123208	132665	2.82%	0.427%
13	11.163	1541	1543	1547	rVB	92834	83788	1.78%	0.270%
14	11.245	1553	1557	1560	rBV	1925842	1493390	31.75%	4.807%
15	11.780	1637	1648	1652	rBV2	102022	200393	4.26%	0.645%
16	12.563	1776	1781	1793	rBV4	99408	222137	4.72%	0.715%
17	12.833	1823	1827	1830	rBV	3847830	3311723	70.41%	10.659%
18	13.792	1984	1990	2001	rBV7	64414	254508	5.41%	0.819%
19	13.880	2001	2005	2017	rVB	1075600	1042490	22.16%	3.355%
20	14.733	2147	2150	2154	rBV	59941	61757	1.31%	0.199%
21	14.986	2190	2193	2196	rBV	63446	64131	1.36%	0.206%
22	15.298	2241	2246	2251	rBV	922918	1093807	23.25%	3.521%
23	15.757	2320	2324	2328	rVB2	63517	83304	1.77%	0.268%
24	16.233	2401	2405	2409	rBV3	36209	58809	1.25%	0.189%

Sum of corrected areas: 31069455

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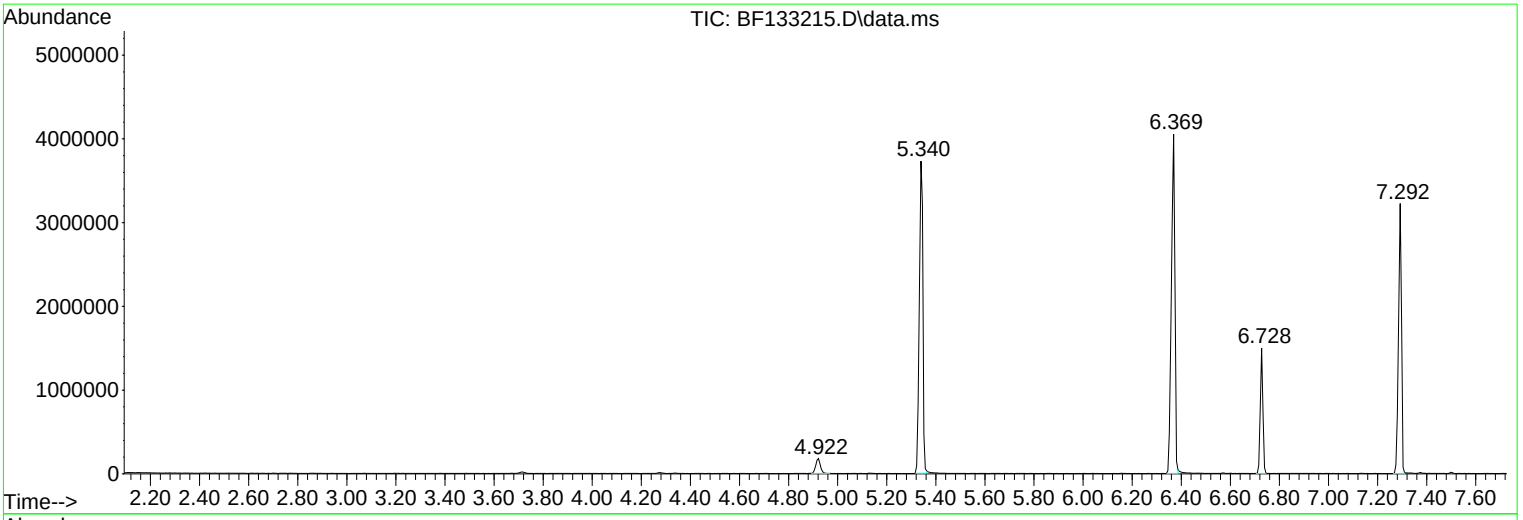
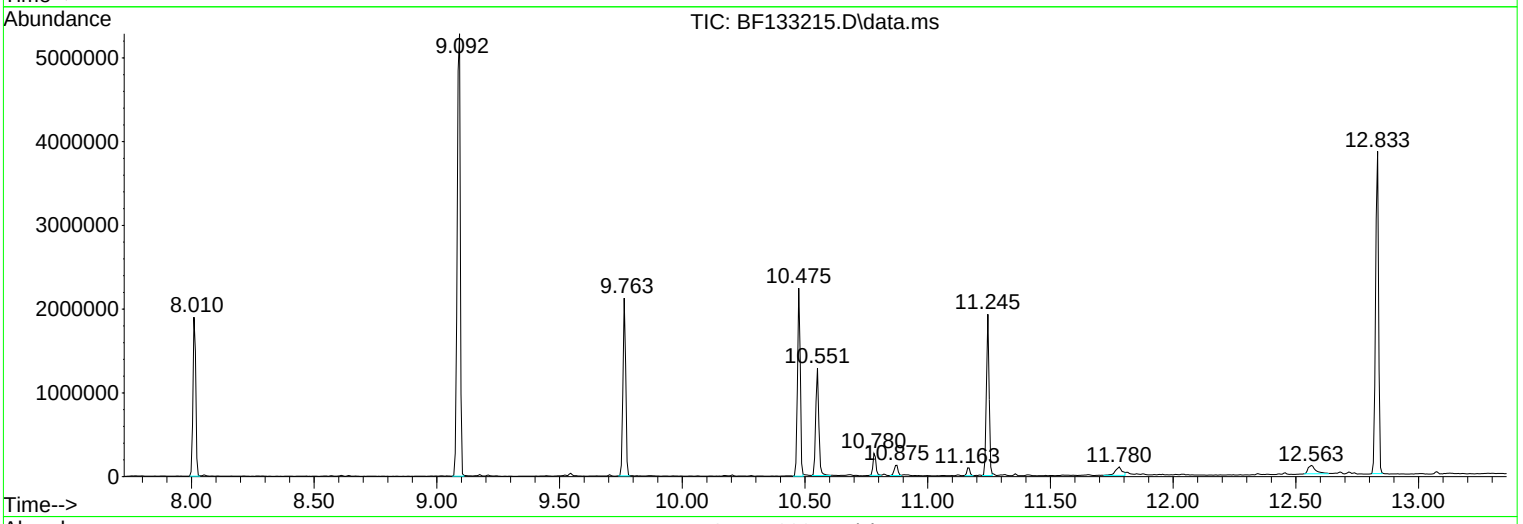
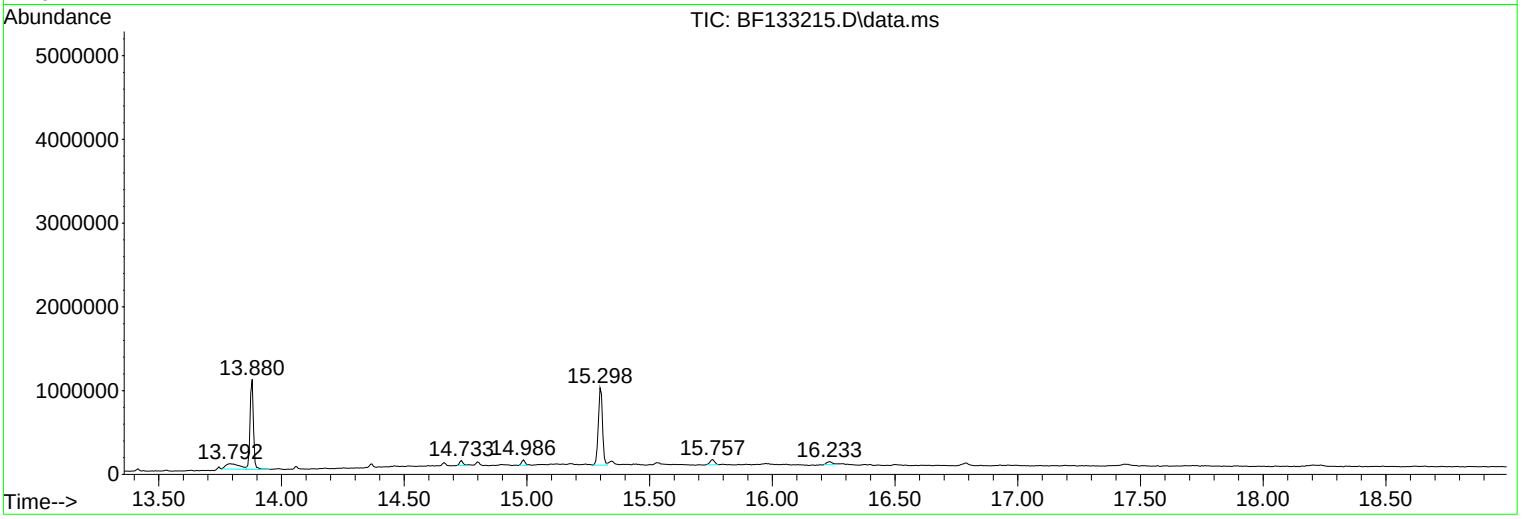
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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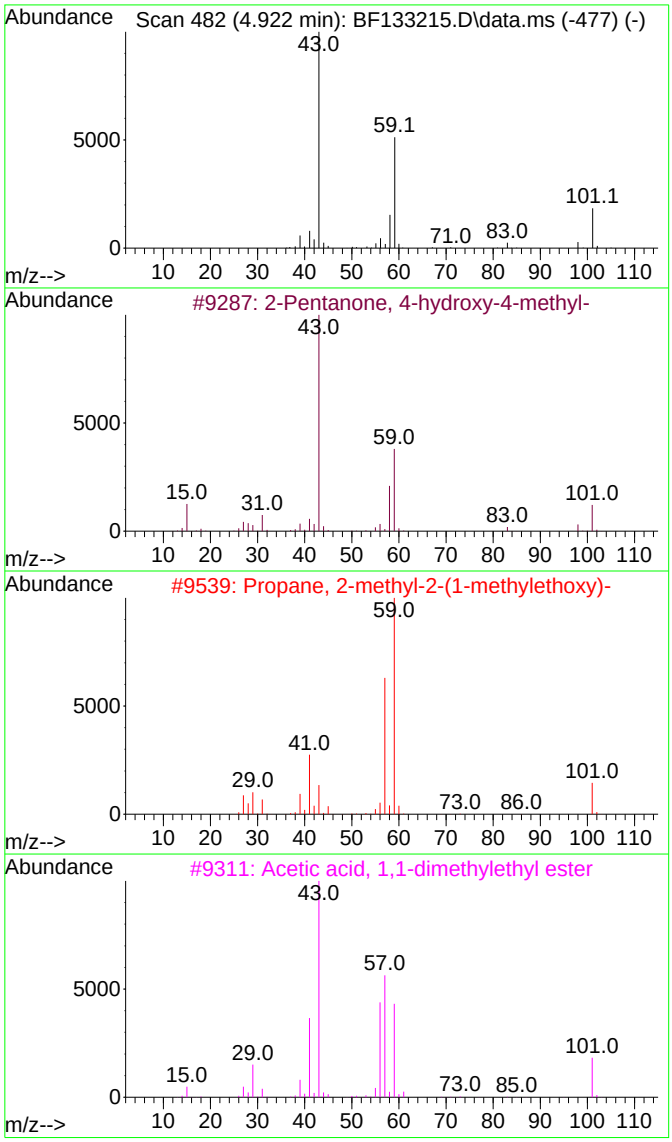
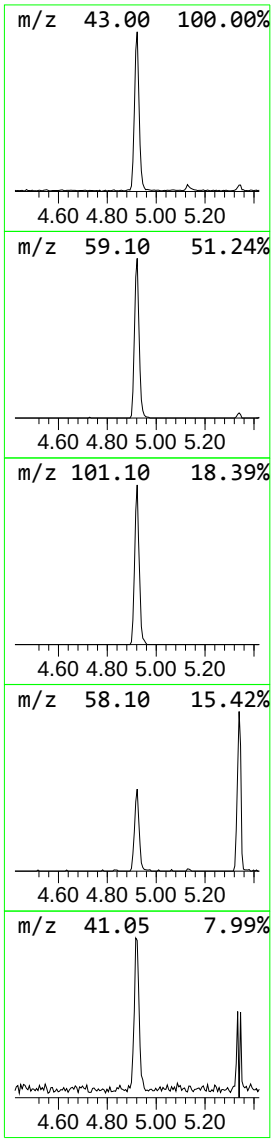
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	4.26 ng	234857	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
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

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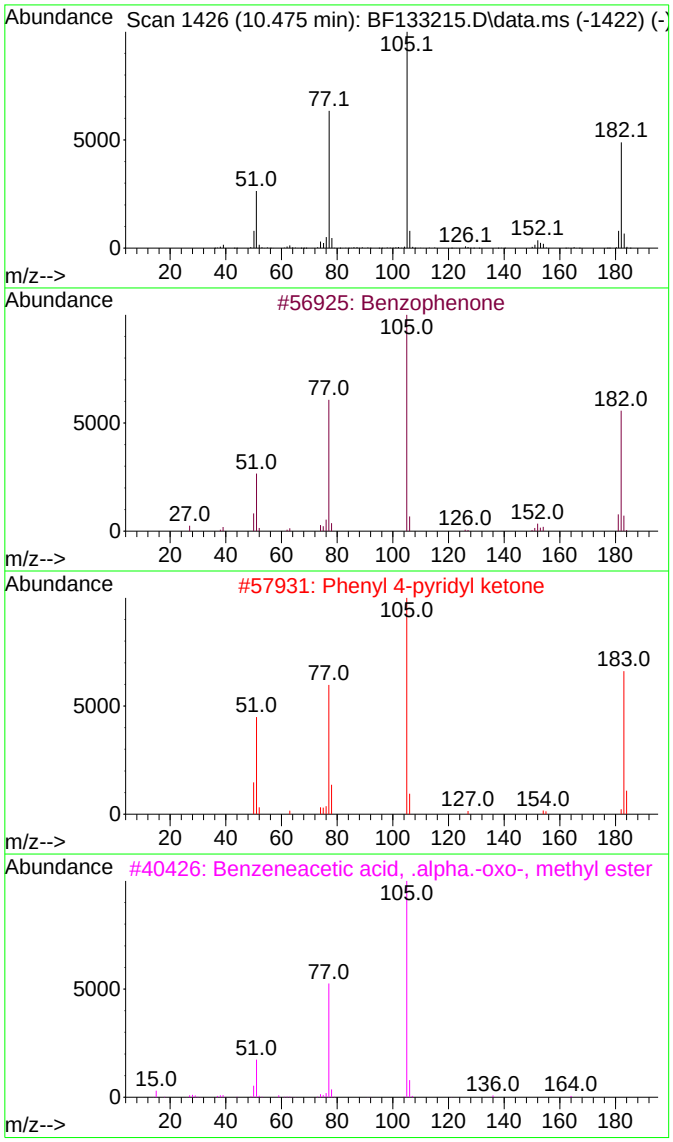
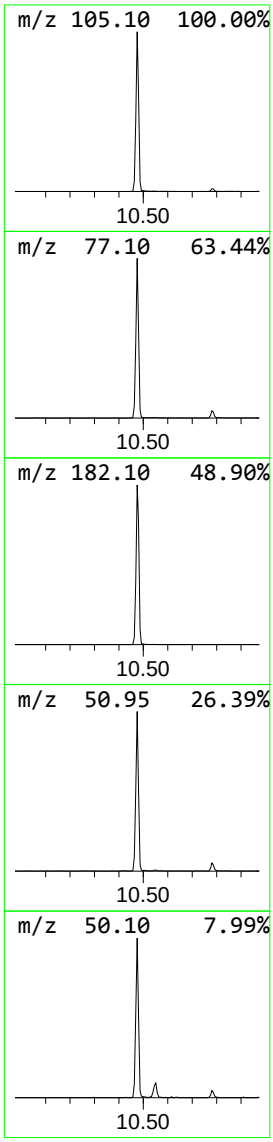
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	21.24 ng	1772910	Acenaphthene-d10	9.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
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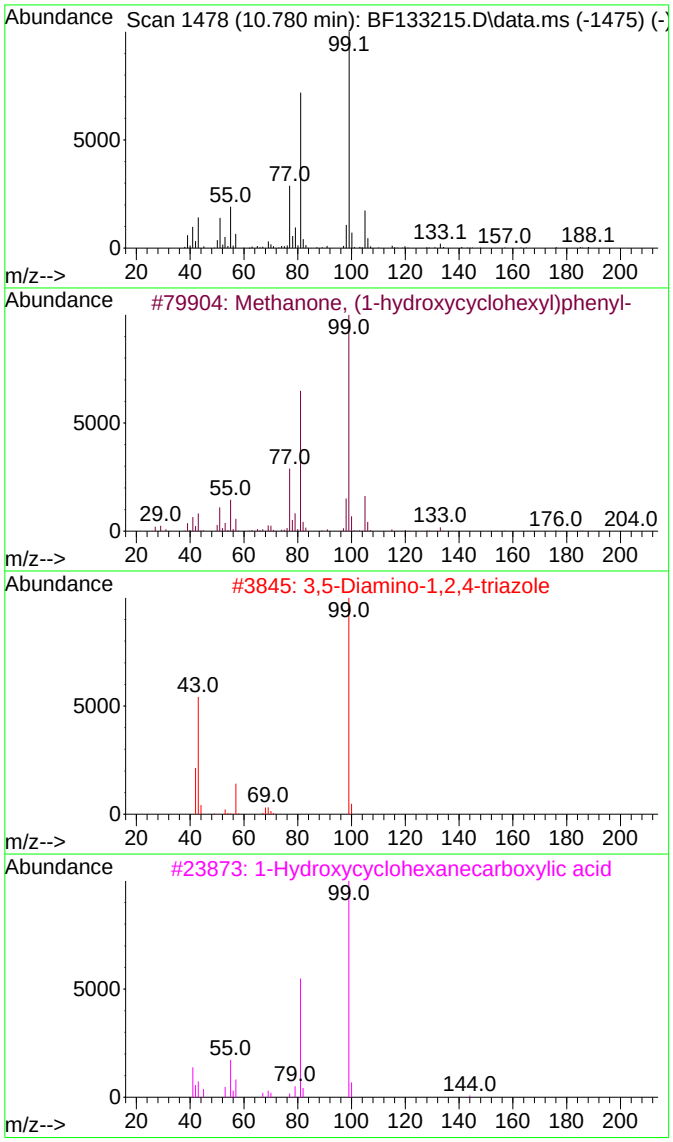
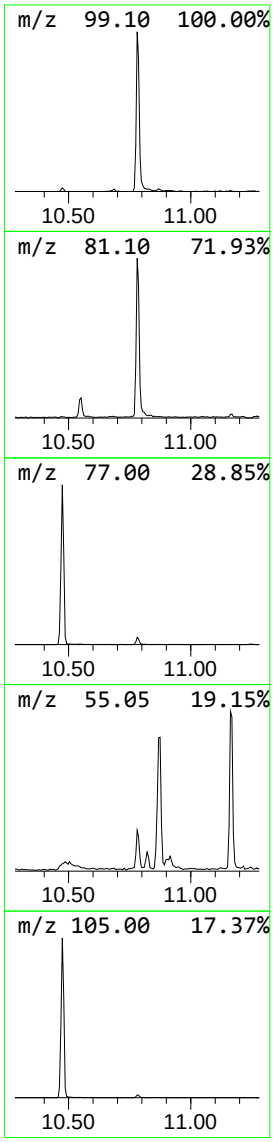
****
Peak Number 3 Methanone, (1-hydroxycycloh... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.780	3.04 ng	226729	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	43
3	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	40
4	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	38
5	Hexanoic acid, thio-, S-butyl ester	188	C10H20OS	002432-79-3	38





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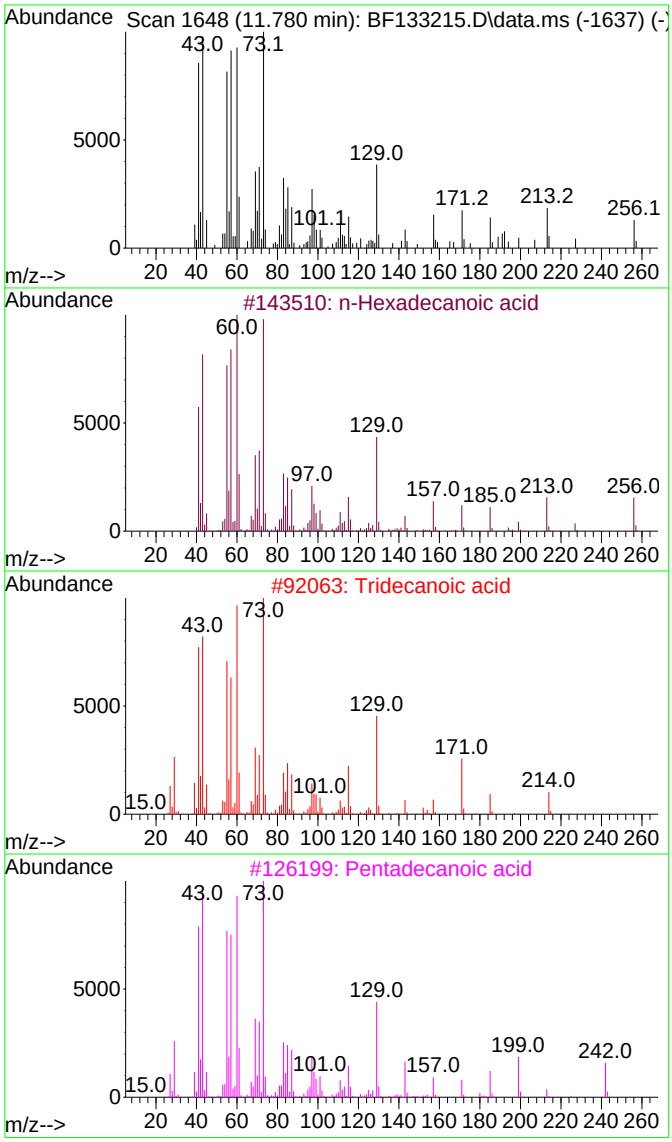
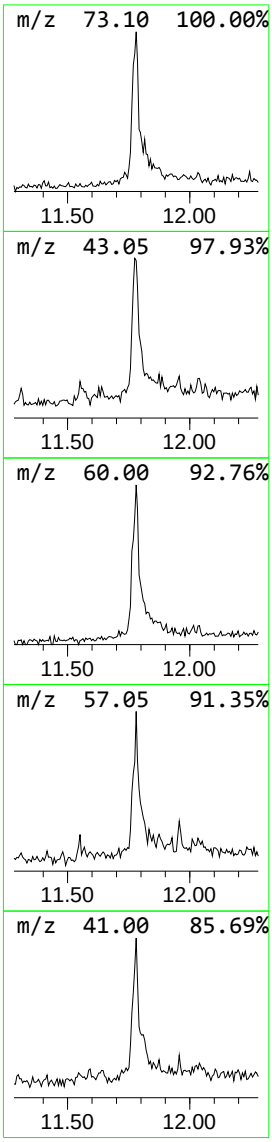
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	2.68 ng	200393	Phenanthrene-d10	11.245

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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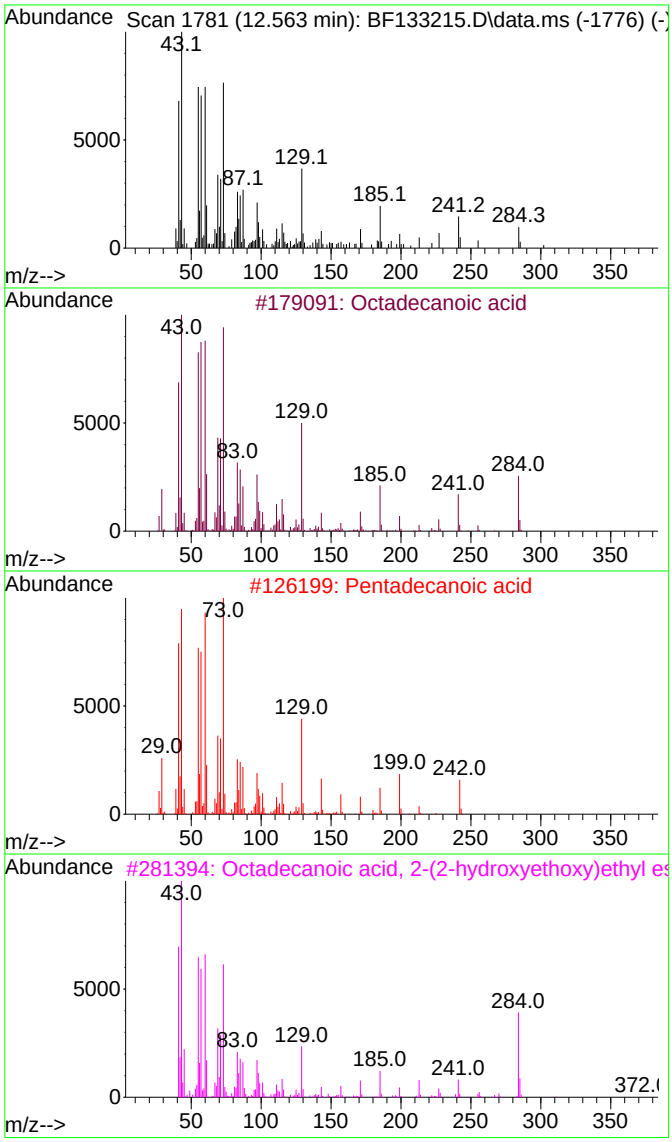
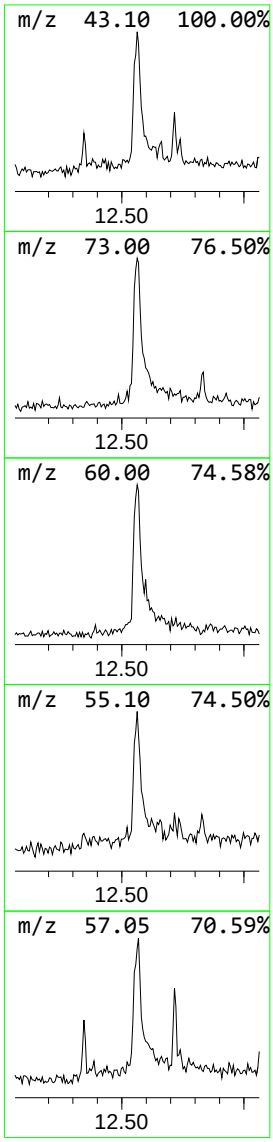
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	2.97 ng	222137	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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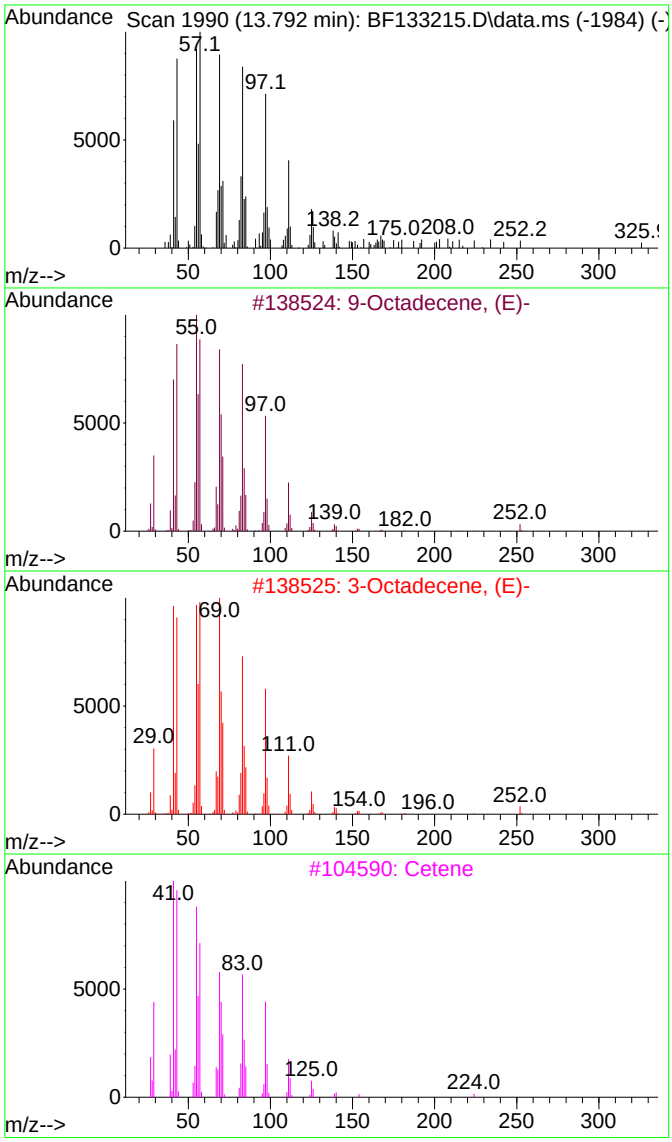
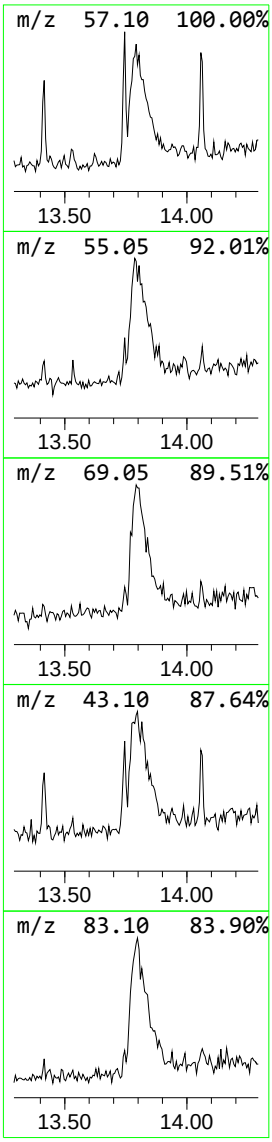
Peak Number 6 9-Octadecene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	4.88 ng	254508	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
2	3-Octadecene, (E)-	252	C18H36	007206-19-1	87
3	Cetene	224	C16H32	000629-73-2	83
4	1-Octadecene	252	C18H36	000112-88-9	83
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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-...	4.922	4.3	ng	234857	1	6.728	1103680	20.0
Benzophenone	10.475	21.2	ng	1772910	3	9.763	1669700	20.0
Methanone, (1-h...	10.780	3.0	ng	226729	4	11.245	1493390	20.0
n-Hexadecanoic ...	11.780	2.7	ng	200393	4	11.245	1493390	20.0
Octadecanoic acid	12.563	3.0	ng	222137	4	11.245	1493390	20.0
9-Octadecene, (E)-	13.792	4.9	ng	254508	5	13.880	1042490	20.0