LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134115.D
Acq On : 07 Jul 2023 01:21
Operator : CG\JU
Sample : 03375-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(8-10)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134115.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	25	rVB	1201264	1651068	65.88%	8.494%
2	2.275	29	32	41	rVB	41942	64838	2.59%	0.334%
3	5.093	507	511	521	rBV	65149	85541	3.41%	0.440%
4	5.481	573	577	580	rBV	2333876	2110979	84.23%	10.860%
5	6.481	742	747	750	rBV	2188176	2165341	86.39%	11.140%
6	6.845	805	809	818	rBV	706750	604827	24.13%	3.112%
7	7.404	900	904	916	rBV	1497828	1437897	57.37%	7.397%
8	8.122	1022	1026	1038	rBV	932177	803671	32.07%	4.135%
9	9.198	1205	1209	1213	rBV	2686955	2506354	100.00%	12.894%
10	9.881	1321	1325	1338	rVB	1079430	875761	34.94%	4.505%
11	10.598	1443	1447	1454	rBV	296125	239412	9.55%	1.232%
12	10.675	1456	1460	1468	rBV	1993597	1774018	70.78%	9.127%
13	11.375	1575	1579	1587	rBV	1126107	931564	37.17%	4.792%
14	11.904	1666	1669	1673	rBV	224840	208781	8.33%	1.074%
15	12.698	1801	1804	1811	rBV2	28936	42831	1.71%	0.220%
16	12.974	1846	1851	1854	rBV	2803564	2476805	98.82%	12.742%
17	13.880	1996	2005	2007	rBV	27959	31289	1.25%	0.161%
18	13.927	2007	2013	2027	rVV4	46312	168914	6.74%	0.869%
19	14.033	2027	2031	2042	rVB	728161	691545	27.59%	3.558%
20	15.533	2281	2286	2297	rBV2	397748	566550	22.60%	2.915%

Sum of corrected areas: 19437986

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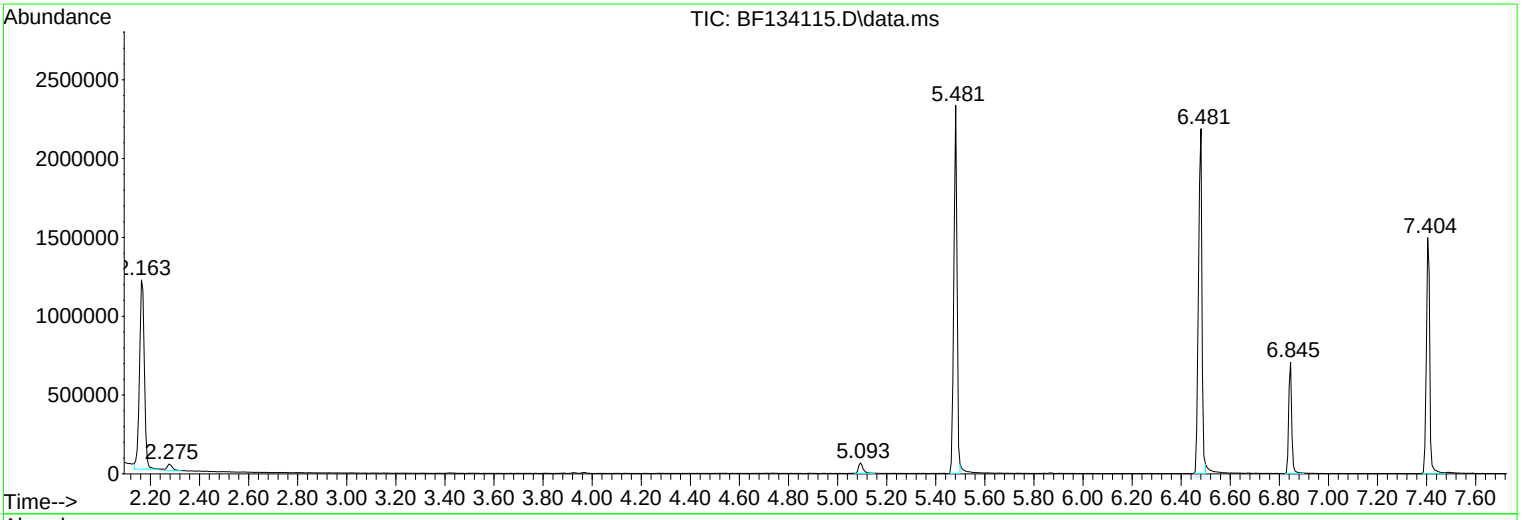
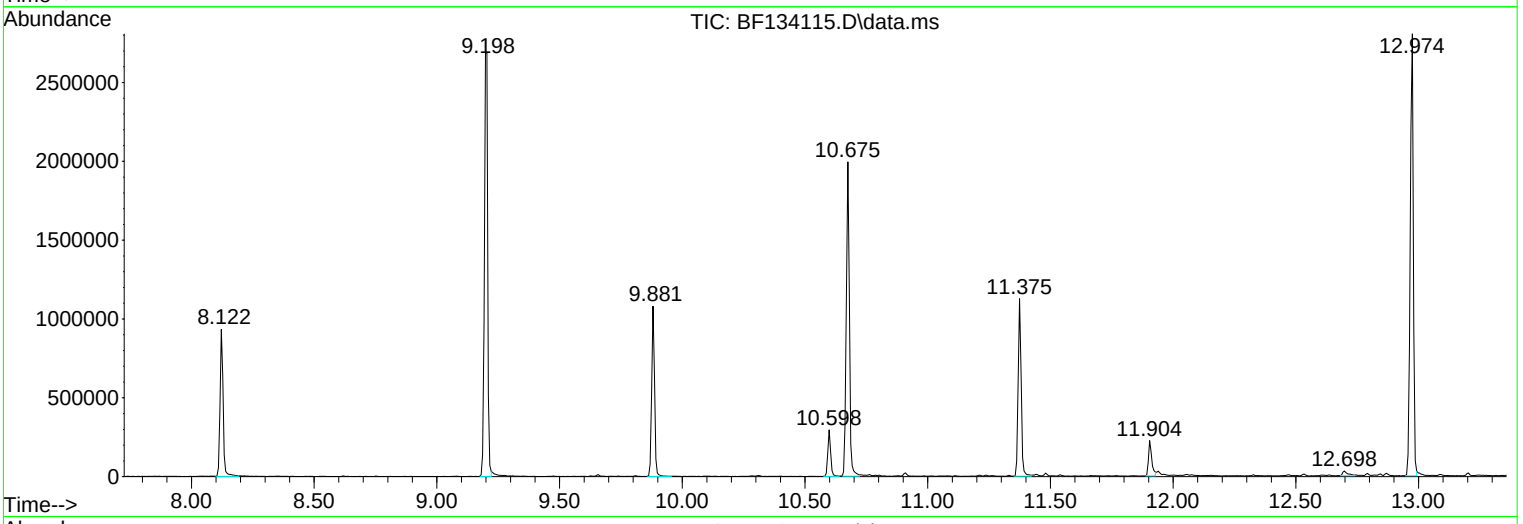
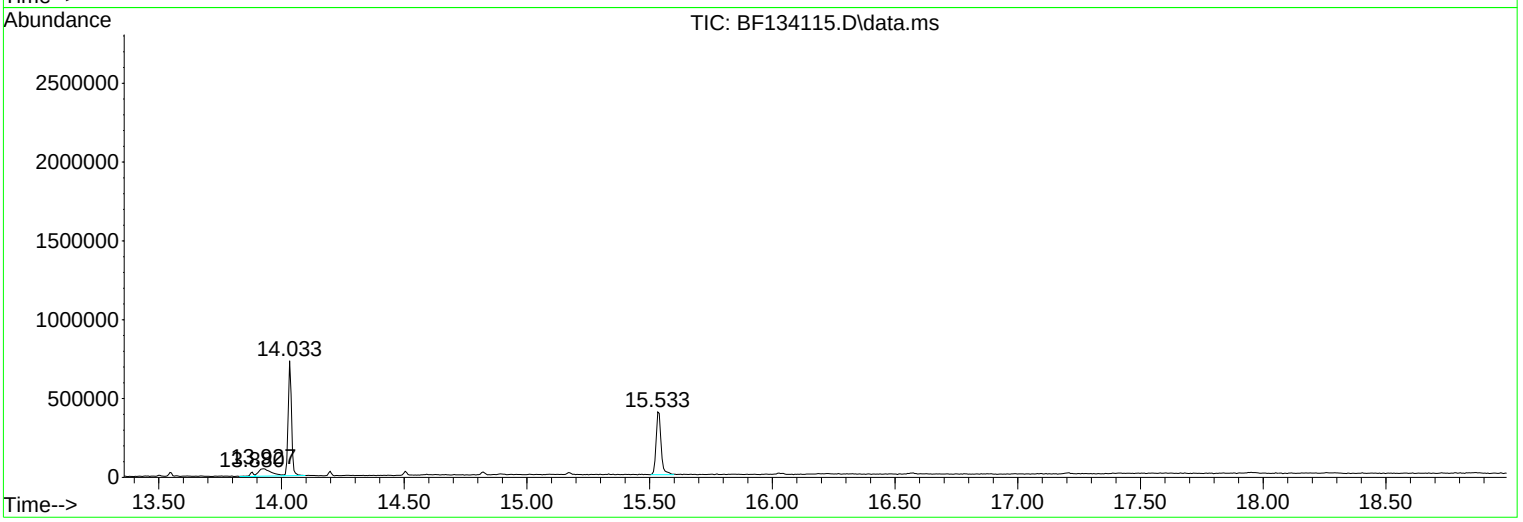
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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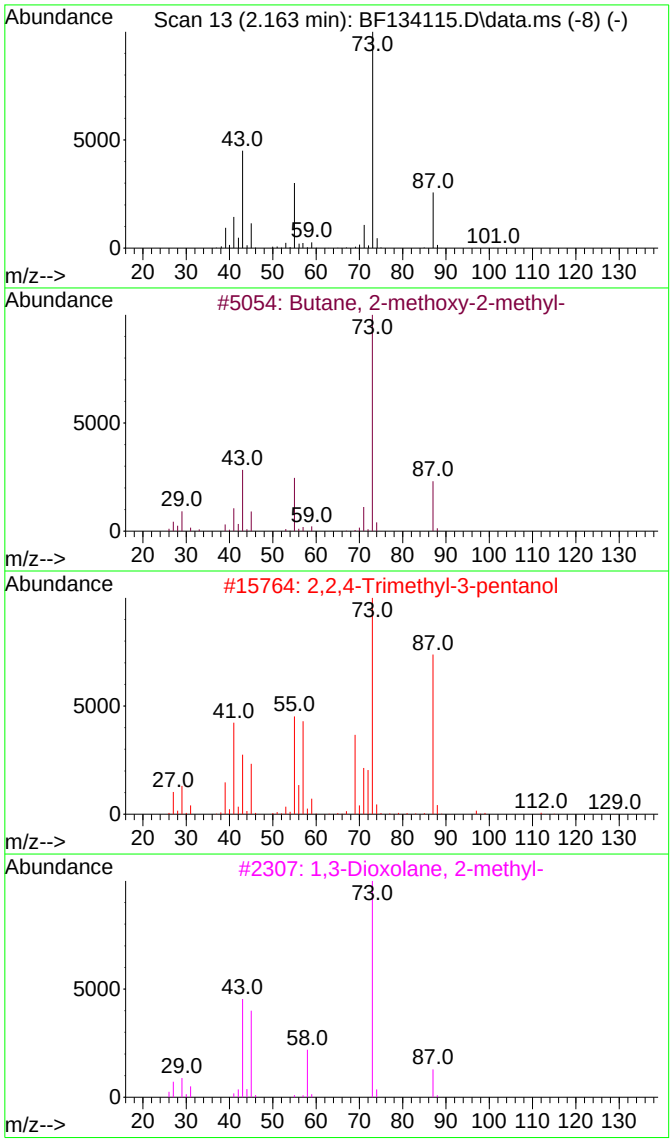
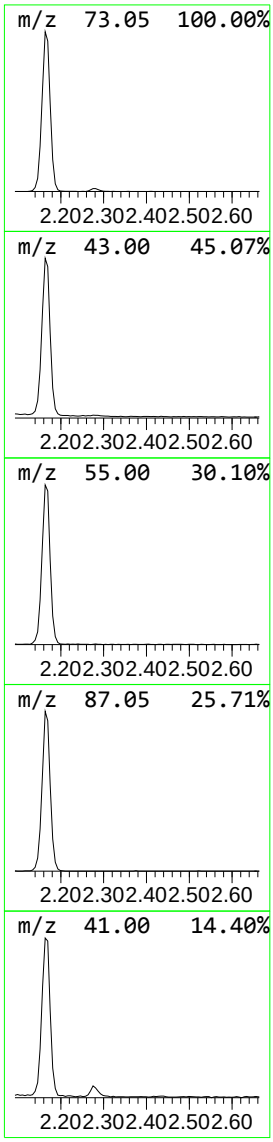
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	54.60 ng	1651070	1,4-Dichlorobenzene-d4	6.845

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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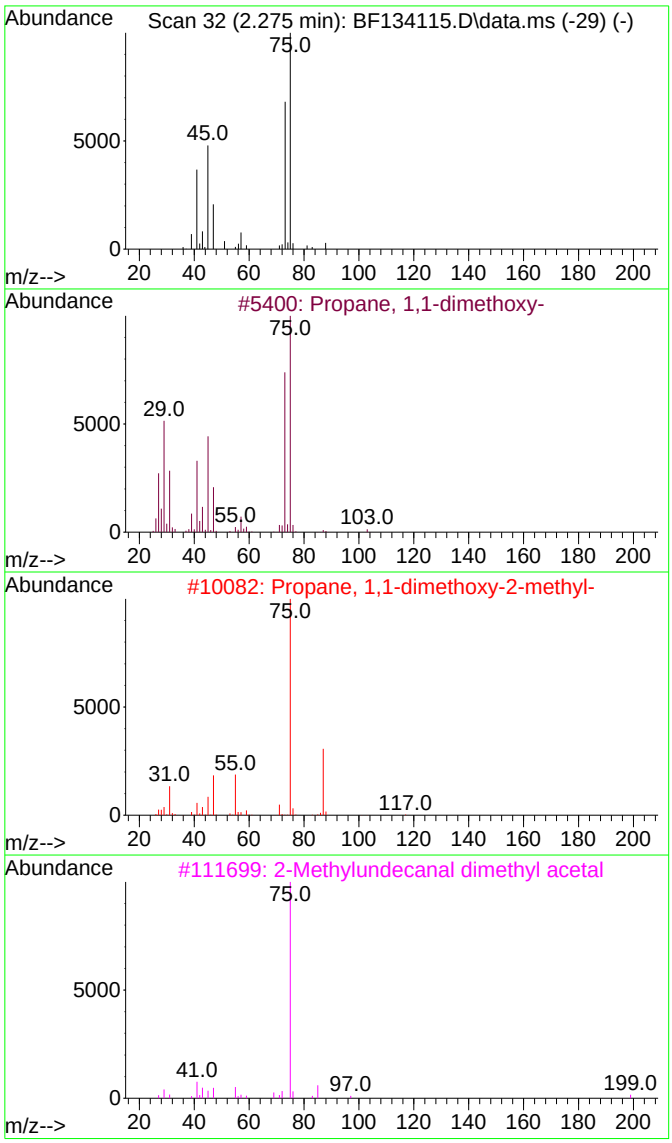
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

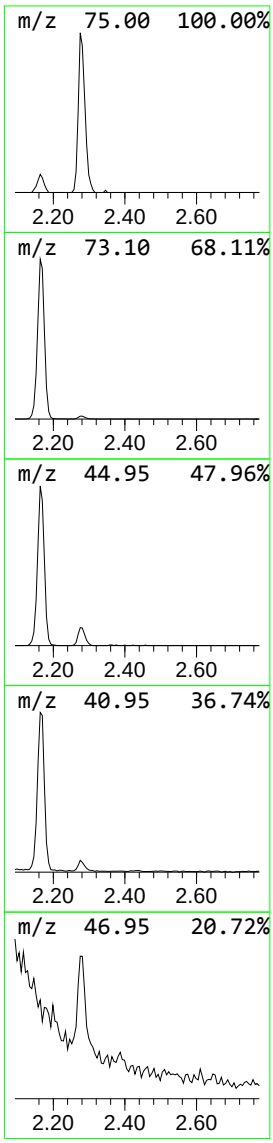
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	2.14 ng	64838	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	33
3	2-Methylundecanal dimethyl acetal	230	C14H30O2	1010430-97-6	25
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9





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Misc :
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Instrument :
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ClientSampleId :
SB-3(8-10)

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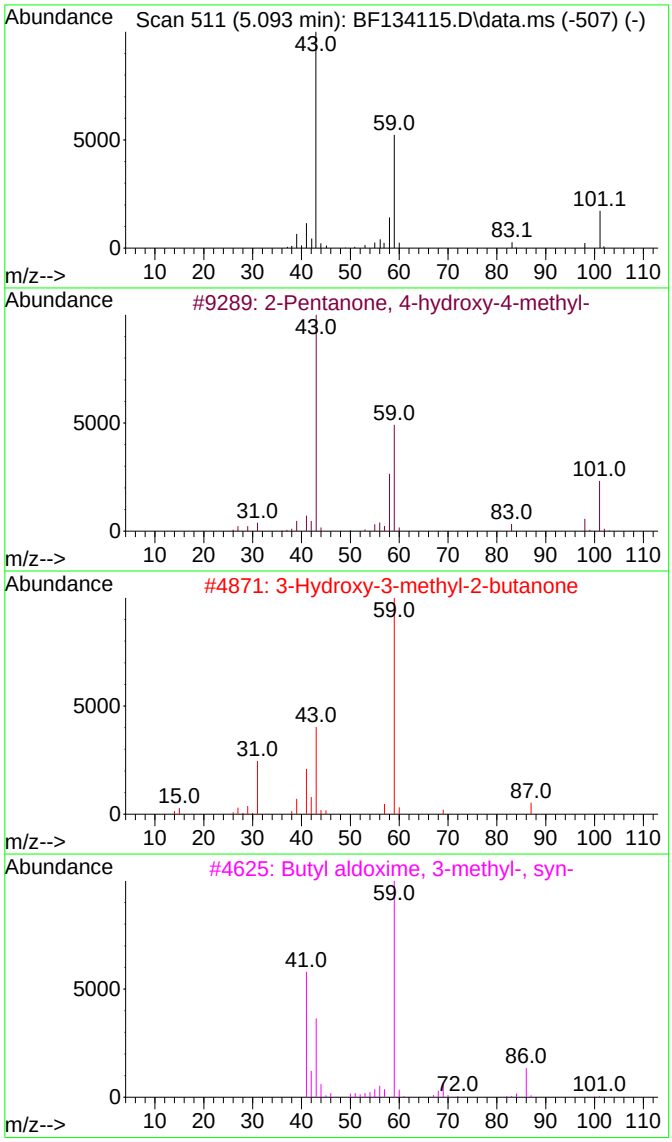
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

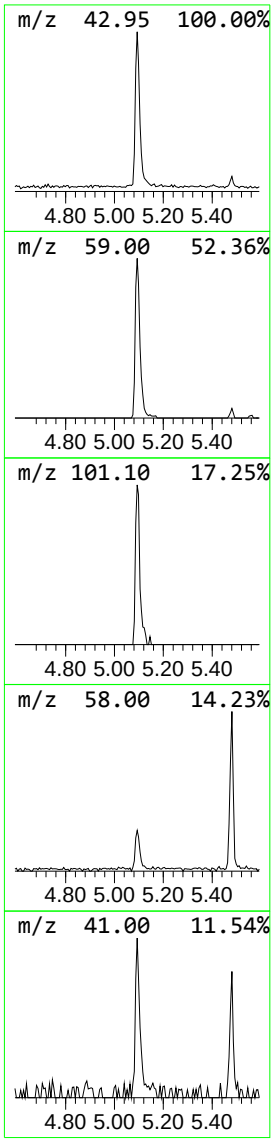
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.83 ng	85541	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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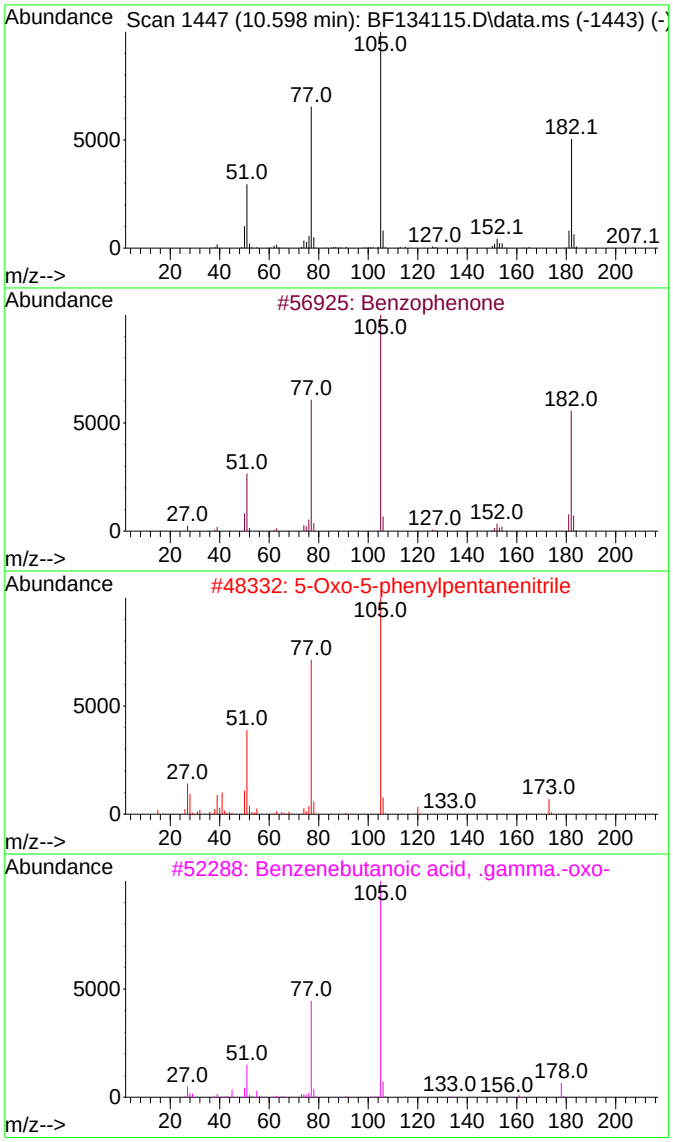
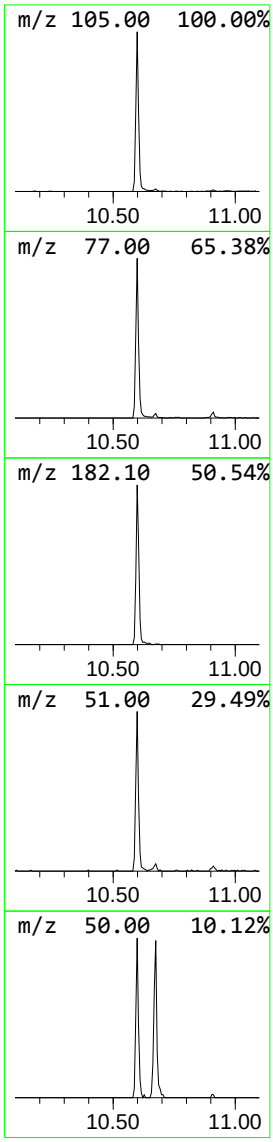
Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	5.47 ng	239412	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	50
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
5	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50





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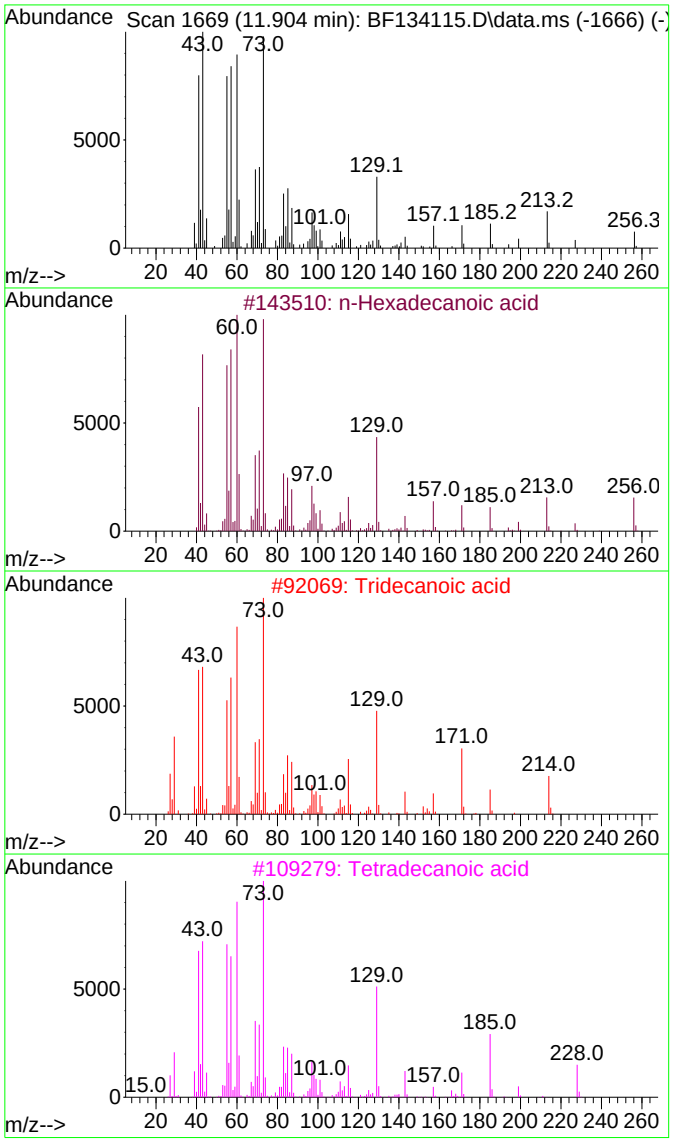
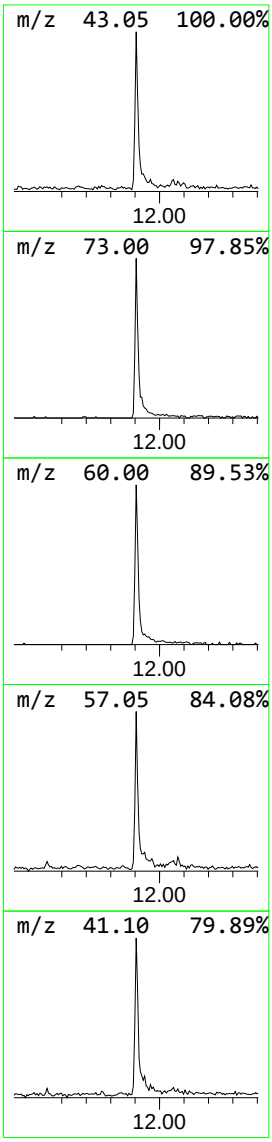
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.48 ng	208781	Phenanthrene-d10	11.375

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	97
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Nonanoic acid	158	C9H18O2	000112-05-0	47





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TIC Integration Parameters: LSCINT.P

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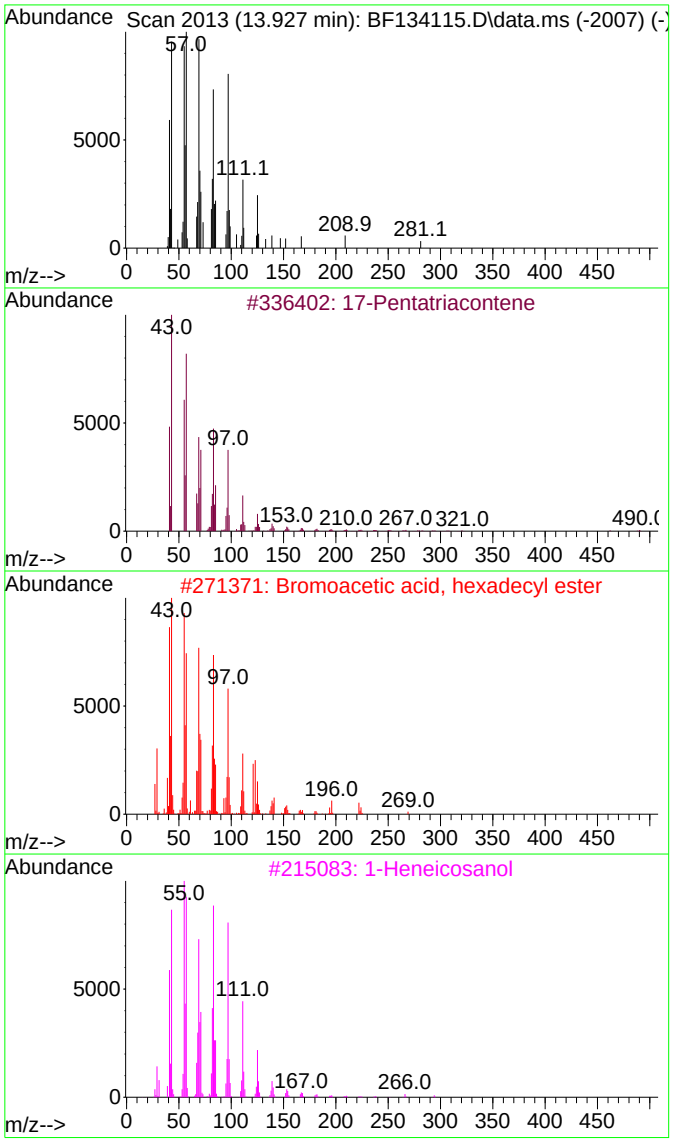
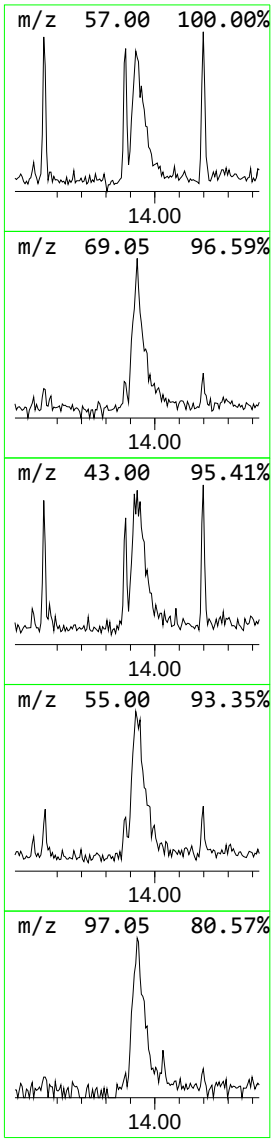
Peak Number 6 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	4.89 ng	168914	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
3	1-Heneicosanol	312	C21H44O	015594-90-8	68
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	64
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	62





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...	2.163	54.6	ng	1651070	1	6.845	604827	20.0
Propane, 1,1-di...	2.275	2.1	ng	64838	1	6.845	604827	20.0
2-Pentanone, 4-...	5.093	2.8	ng	85541	1	6.845	604827	20.0
Benzophenone	10.598	5.5	ng	239412	3	9.881	875761	20.0
n-Hexadecanoic ...	11.904	4.5	ng	208781	4	11.375	931564	20.0
17-Pentatriacon...	13.927	4.9	ng	168914	5	14.033	691545	20.0