LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134105.D
Acq On : 06 Jul 2023 19:28
Operator : CG\JU
Sample : 03486-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BAYONNE-COMP

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: BF134105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	25	rVB	1135429	1541247	66.70%	8.692%
2	2.281	29	33	43	rVB2	34542	57377	2.48%	0.324%
3	5.087	507	510	522	rVB	115761	156785	6.79%	0.884%
4	5.481	573	577	594	rBV	2134975	2078162	89.94%	11.720%
5	6.481	742	747	750	rBV	2167337	2031064	87.90%	11.454%
6	6.846	805	809	818	rBV	625987	504623	21.84%	2.846%
7	7.404	900	904	916	rBV	1372966	1338349	57.92%	7.548%
8	8.122	1023	1026	1039	rBV	791604	651790	28.21%	3.676%
9	9.198	1205	1209	1213	rBV	2539143	2310621	100.00%	13.031%
10	9.881	1321	1325	1334	rBV	858186	716721	31.02%	4.042%
11	10.598	1443	1447	1456	rBV	343570	279069	12.08%	1.574%
12	10.675	1456	1460	1473	rBV	1867709	1622253	70.21%	9.149%
13	10.910	1497	1500	1507	rBV	38195	36605	1.58%	0.206%
14	11.375	1575	1579	1587	rBV	885281	750074	32.46%	4.230%
15	11.904	1666	1669	1678	rBV2	163295	177518	7.68%	1.001%
16	12.622	1785	1791	1795	rBV5	15622	24877	1.08%	0.140%
17	12.698	1801	1804	1814	rBV3	23393	31579	1.37%	0.178%
18	12.975	1846	1851	1854	rBV	2547151	2196142	95.05%	12.385%
19	13.922	2007	2012	2025	rBV4	54794	178326	7.72%	1.006%
20	14.033	2027	2031	2041	rVB	624277	591504	25.60%	3.336%
21	15.539	2282	2287	2298	rBV	337220	457634	19.81%	2.581%

Sum of corrected areas: 17732320

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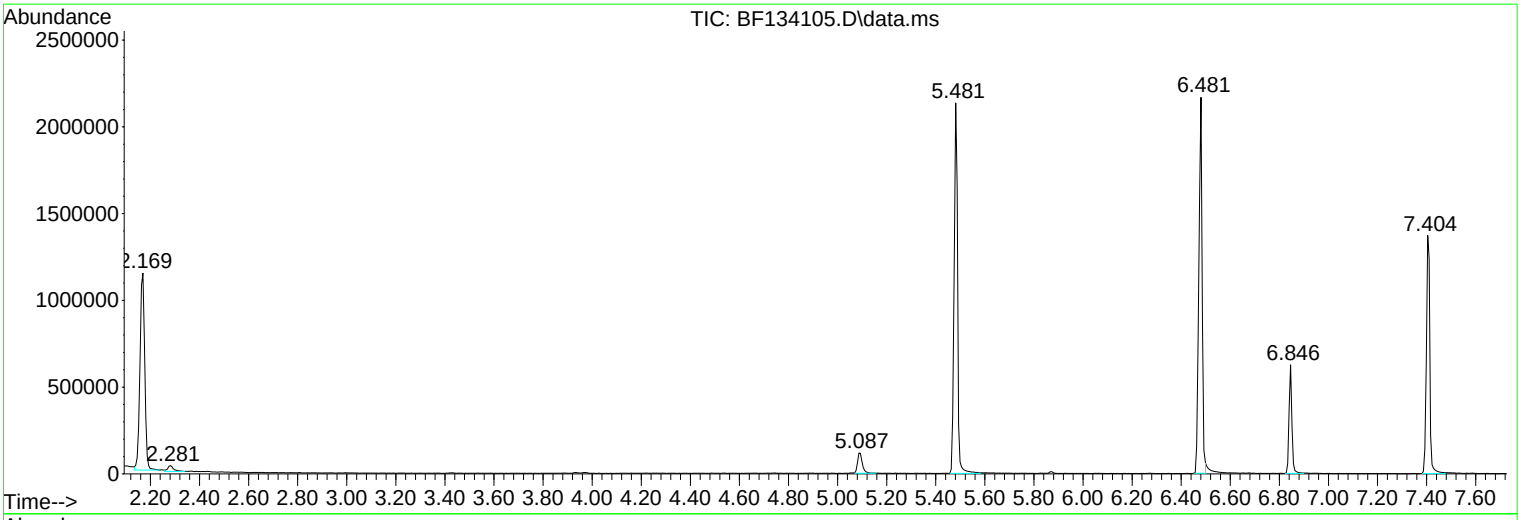
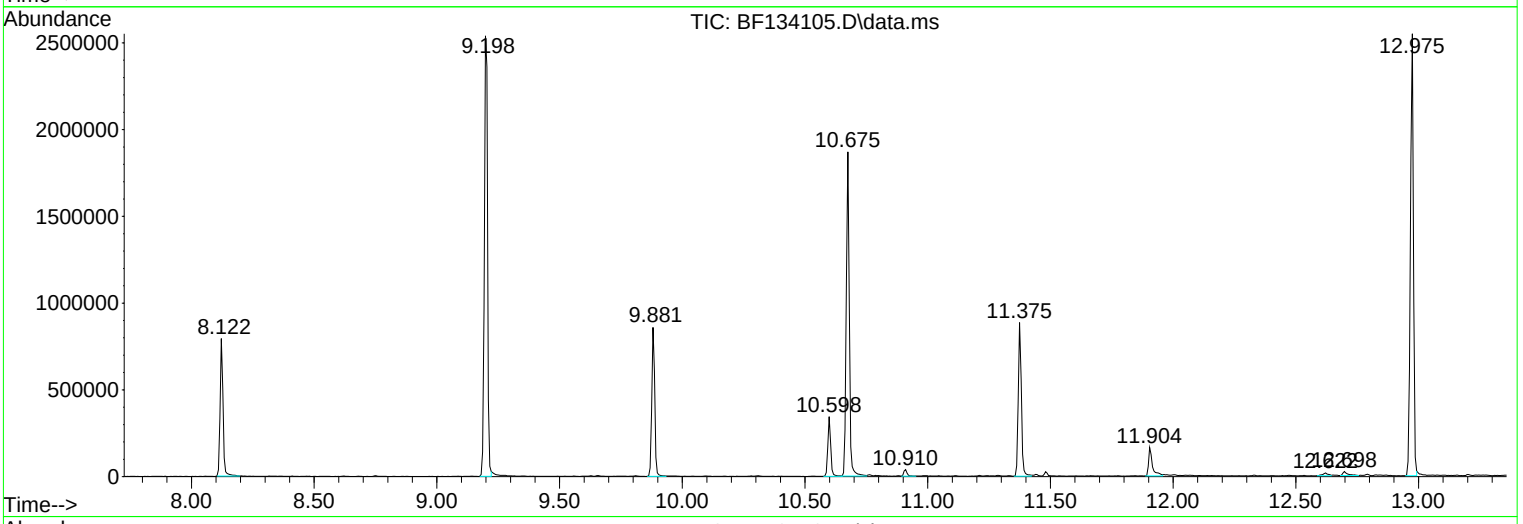
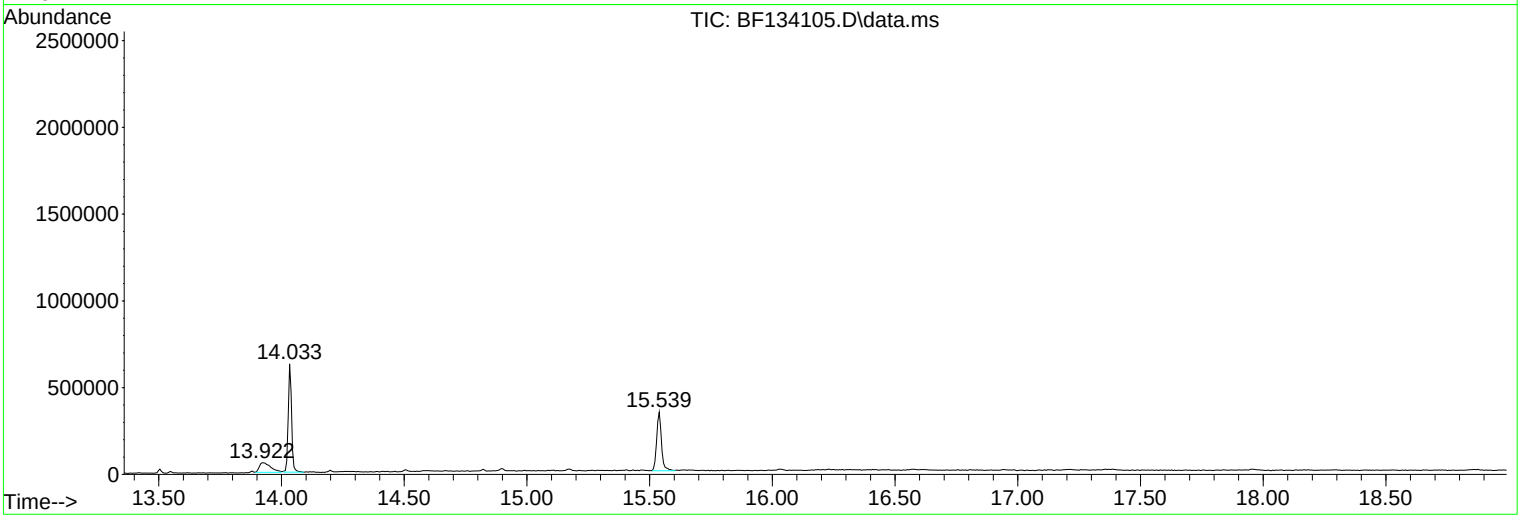
ClientSampleId :
BAYONNE-COMP

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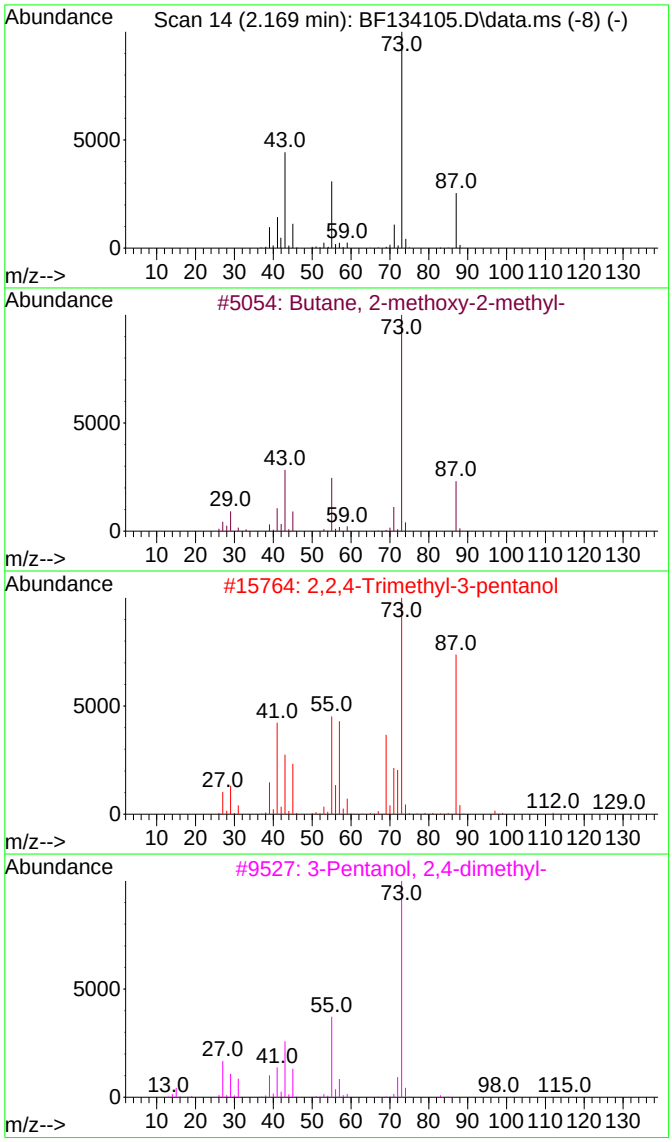
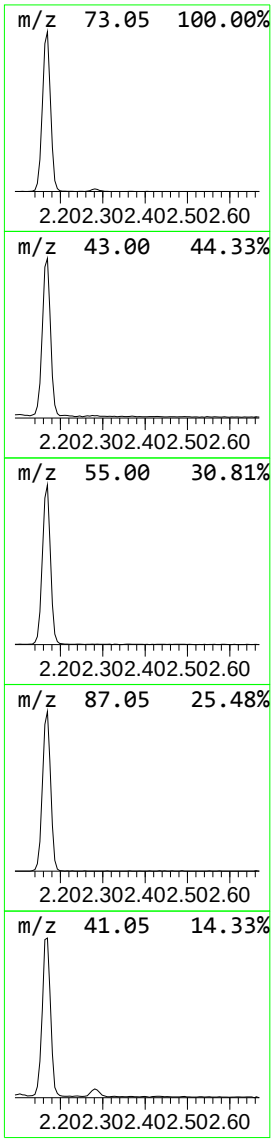
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	61.09 ng	1541250	1,4-Dichlorobenzene-d4	6.846

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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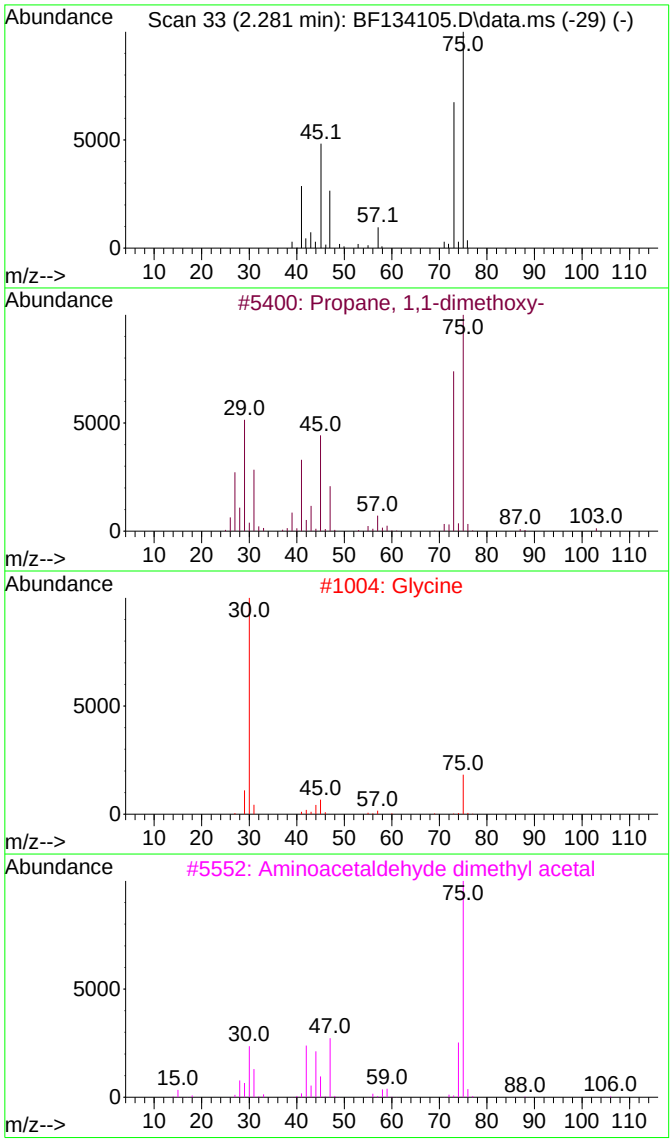
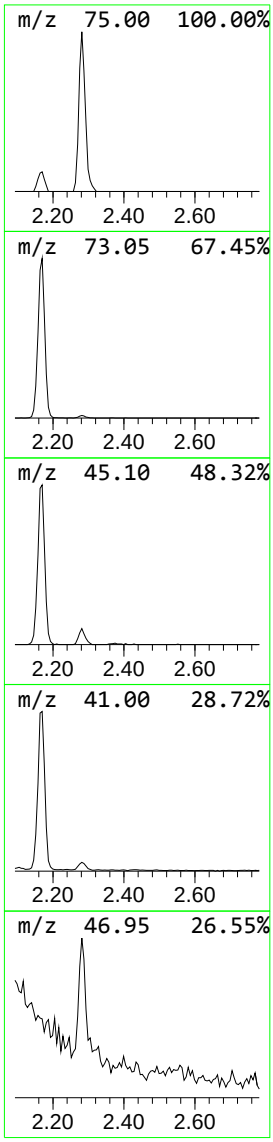
Peak Number 2 unknown2.281 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.27 ng	57377	1,4-Dichlorobenzene-d4	6.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
2	Glycine	75	C2H5NO2	000056-40-6	9
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9





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ALS Vial : 6 Sample Multiplier: 1

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BNA_F
ClientSampleId :
BAYONNE-COMP

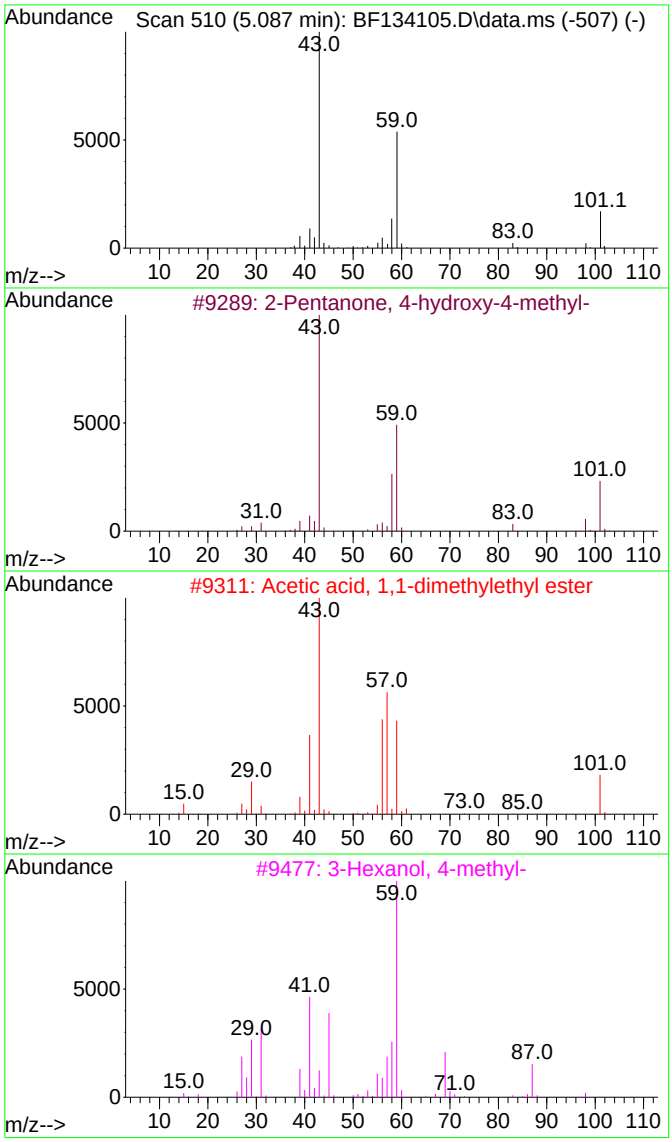
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

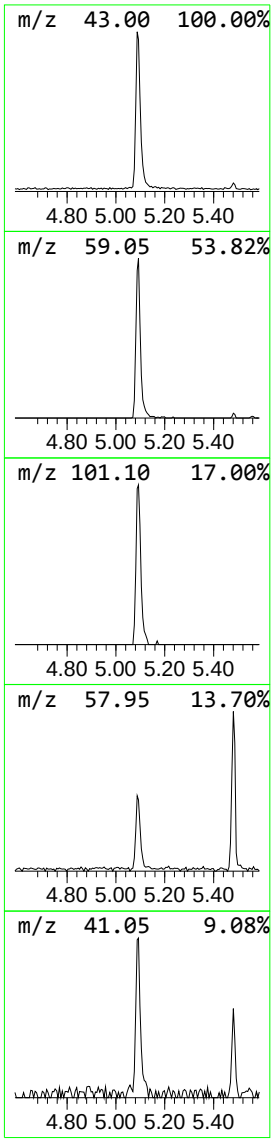
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	6.21 ng	156785	1,4-Dichlorobenzene-d4	6.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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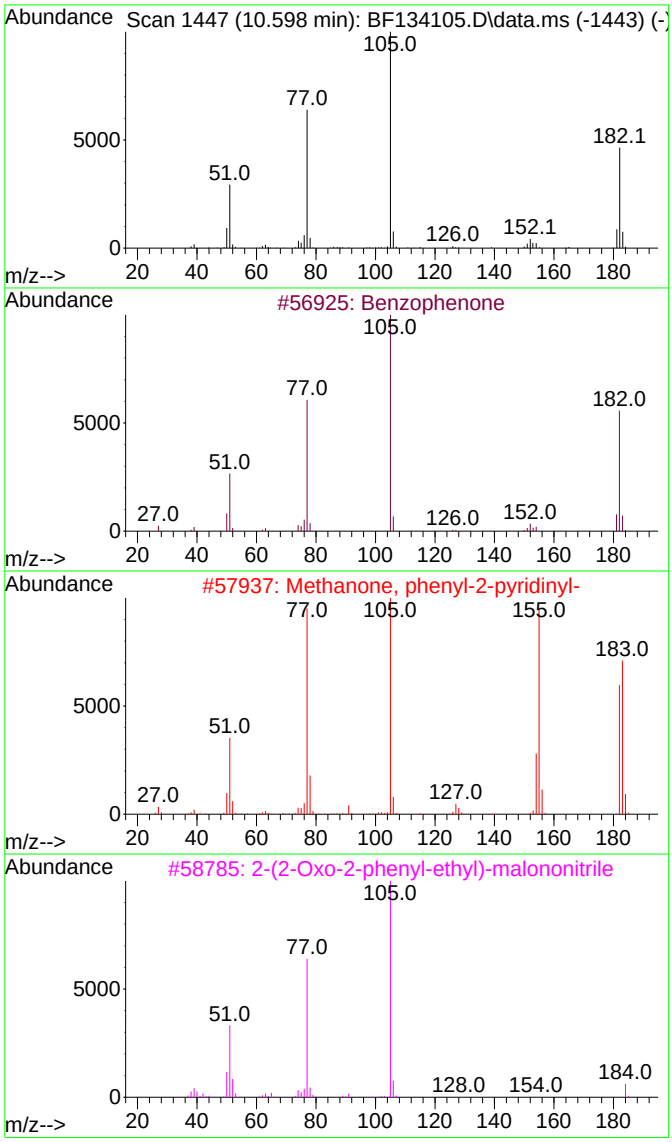
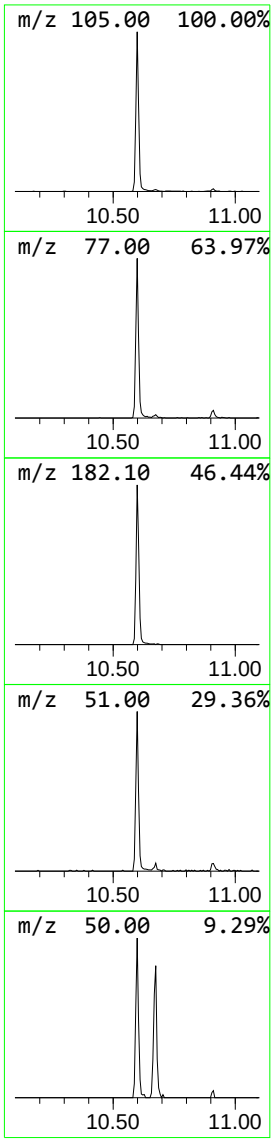
Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	7.79 ng	279069	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	78
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
5	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	50





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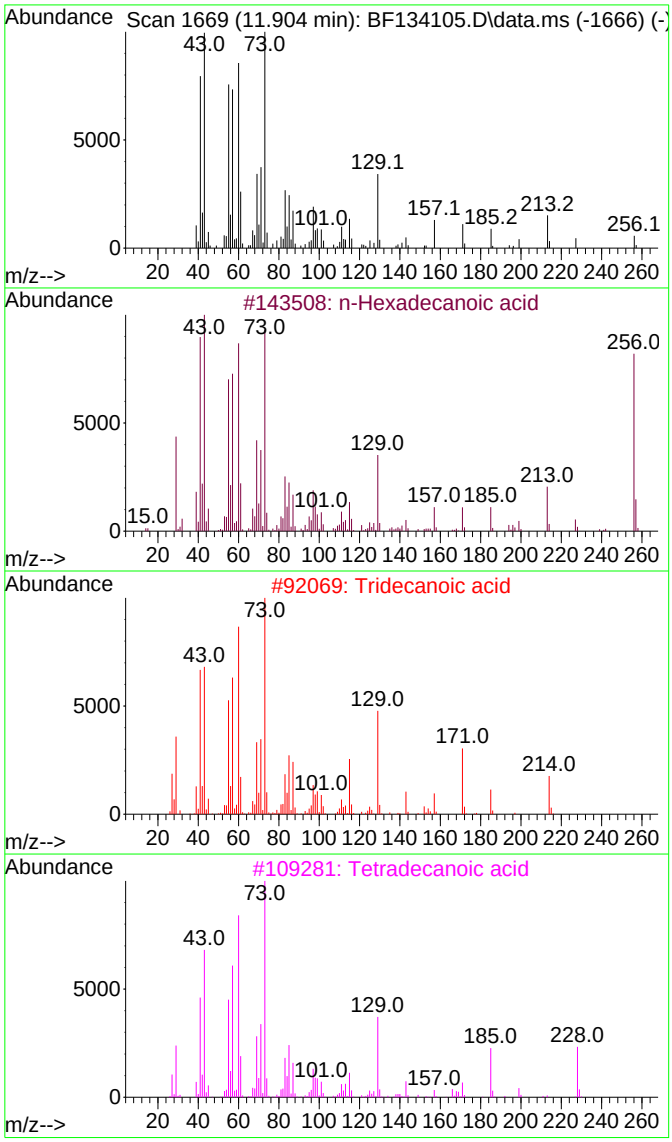
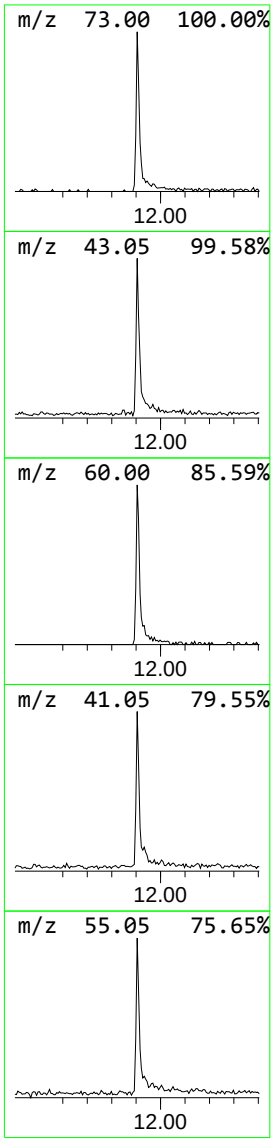
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.73 ng	177518	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	25
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	15





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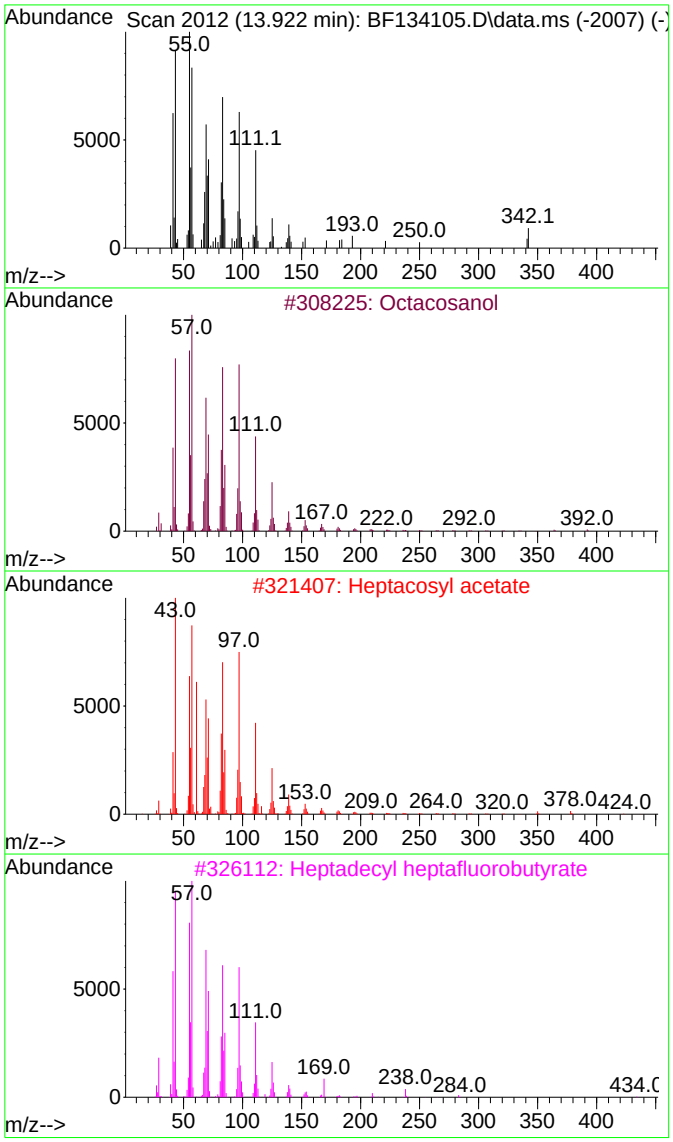
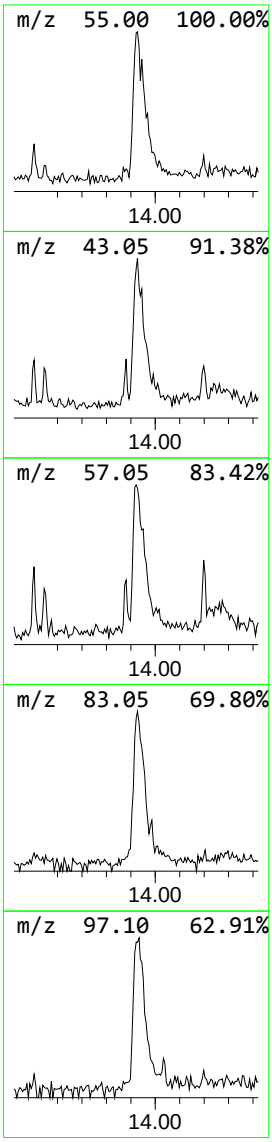
Peak Number 6 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	6.03 ng	178326	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	83
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	76
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	76





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	61.1	ng	1541250	1	6.846	504623	20.0
unknown2.281	2.281	2.3	ng	57377	1	6.846	504623	20.0
2-Pentanone, 4-...	5.087	6.2	ng	156785	1	6.846	504623	20.0
Benzophenone	10.598	7.8	ng	279069	3	9.881	716721	20.0
n-Hexadecanoic ...	11.904	4.7	ng	177518	4	11.375	750074	20.0
Octacosanol	13.922	6.0	ng	178326	5	14.033	591504	20.0