LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
Data File : BF125450.D
Acq On : 13 Sep 2021 18:35
Operator : JU/CG
Sample : M3684-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A008015

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125450.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	27	rBV	1245972	1641623	48.19%	5.888%
2	2.305	32	37	47	rVB	50942	69485	2.04%	0.249%
3	5.110	510	514	527	rVB	220399	265021	7.78%	0.951%
4	5.510	578	582	600	rBV	2948930	3057779	89.77%	10.967%
5	6.522	749	754	757	rBV	3059081	2954477	86.74%	10.597%
6	6.881	812	815	819	rBV	1002026	922797	27.09%	3.310%
7	7.445	906	911	923	rBV	1879658	2020425	59.31%	7.247%
8	8.081	1014	1019	1029	rBV4	60997	185033	5.43%	0.664%
9	8.169	1029	1034	1050	rVB	1313249	1258826	36.96%	4.515%
10	9.245	1211	1217	1220	rBV	3792491	3399941	99.81%	12.195%
11	9.928	1328	1333	1336	rBV	1530088	1367565	40.15%	4.905%
12	10.716	1463	1467	1477	rBV	2490738	2324932	68.25%	8.339%
13	11.416	1582	1586	1589	rBV	1732784	1456482	42.76%	5.224%
14	11.933	1670	1674	1679	rBV	186187	210375	6.18%	0.755%
15	12.633	1789	1793	1798	rBV	138217	123213	3.62%	0.442%
16	12.722	1803	1808	1814	rBV2	82626	101490	2.98%	0.364%
17	12.863	1826	1832	1836	rBV	127767	134950	3.96%	0.484%
18	13.004	1851	1856	1859	rBV	3927148	3406290	100.00%	12.217%
19	13.951	2011	2017	2019	rBV3	41115	75183	2.21%	0.270%
20	14.063	2031	2036	2039	rBV	1320559	1196105	35.11%	4.290%
21	14.086	2039	2040	2050	rVB	81263	66046	1.94%	0.237%
22	15.121	2211	2216	2219	rBV	48700	78582	2.31%	0.282%
23	15.492	2275	2279	2283	rBV	34633	42641	1.25%	0.153%
24	15.557	2285	2290	2302	rBV	711913	909700	26.71%	3.263%
25	16.257	2403	2409	2413	rBV2	181358	327465	9.61%	1.175%
26	16.304	2413	2417	2431	rVB	114232	284206	8.34%	1.019%

Sum of corrected areas: 27880632

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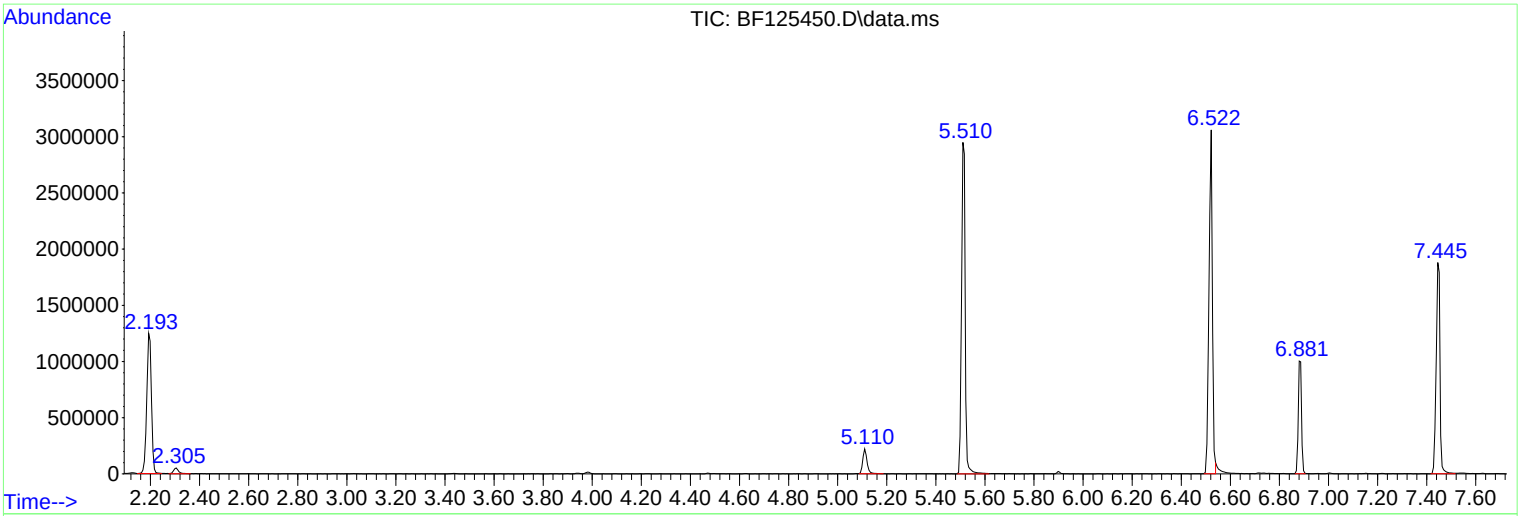
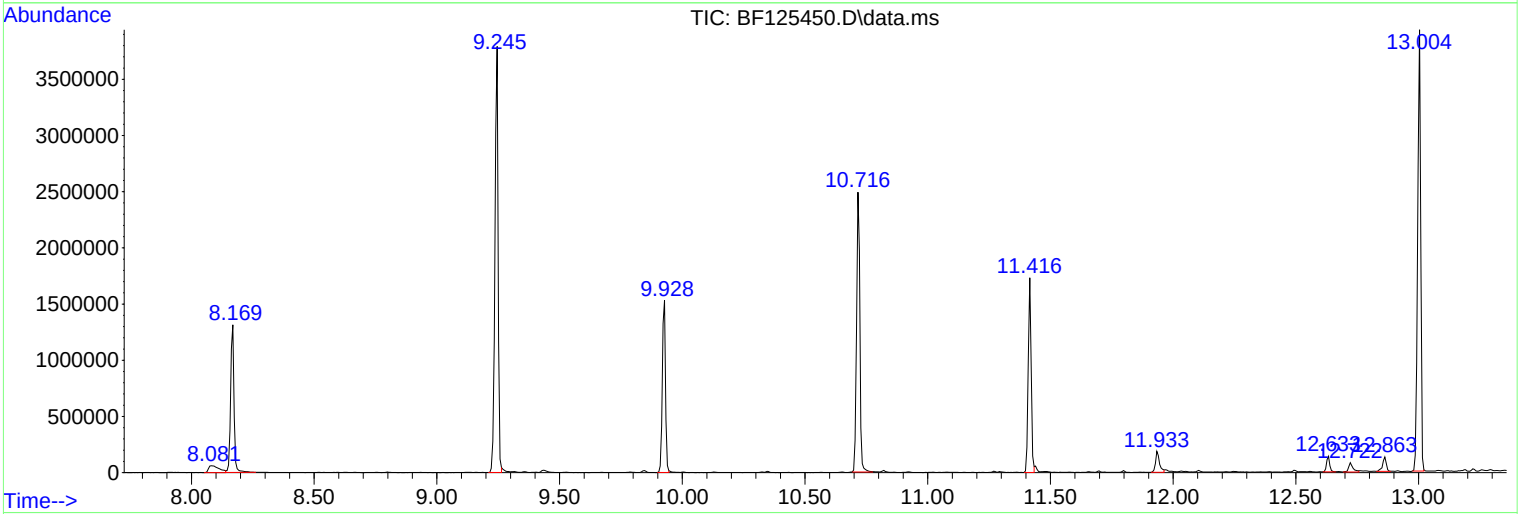
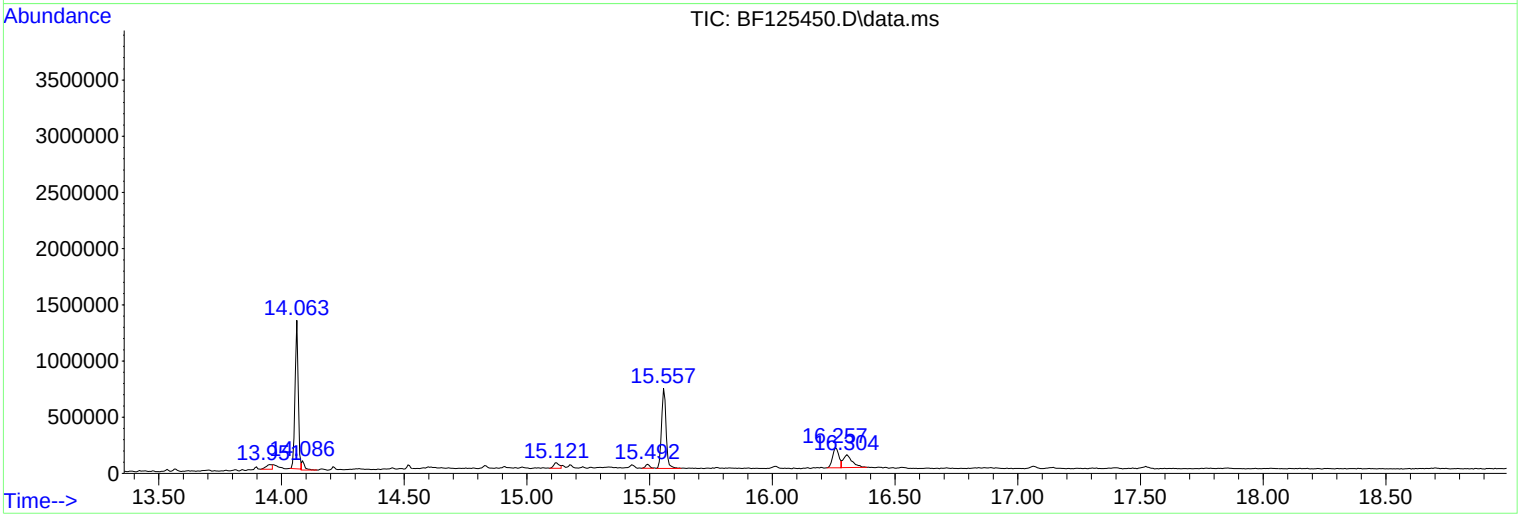
ClientSampleId :
A008015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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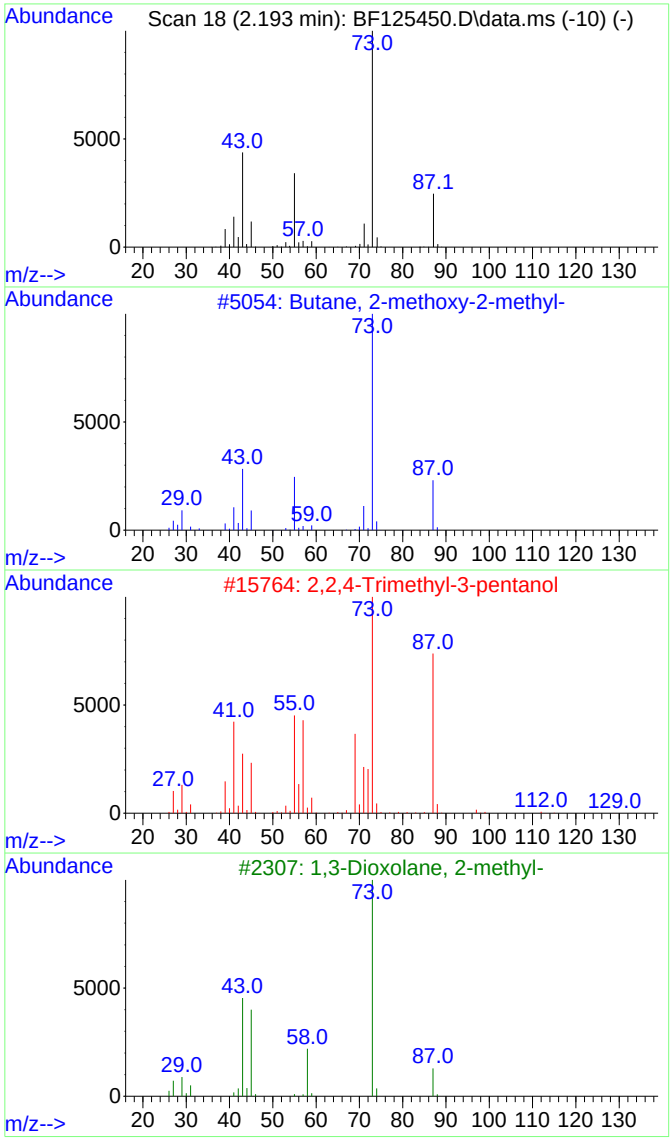
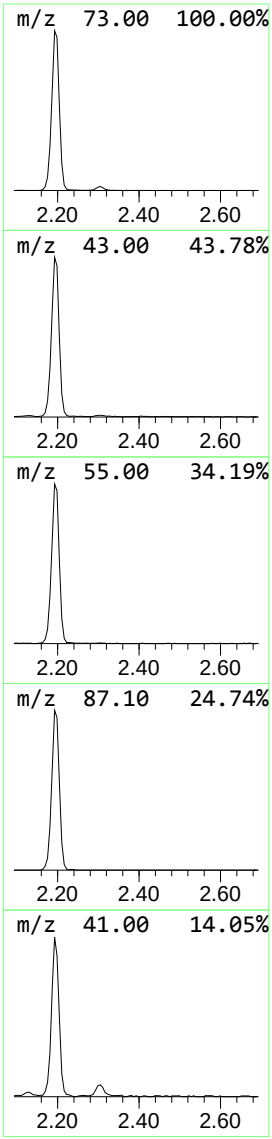
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	35.58 ng	1641620	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23





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Operator : JU/CG
Sample : M3684-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A008015

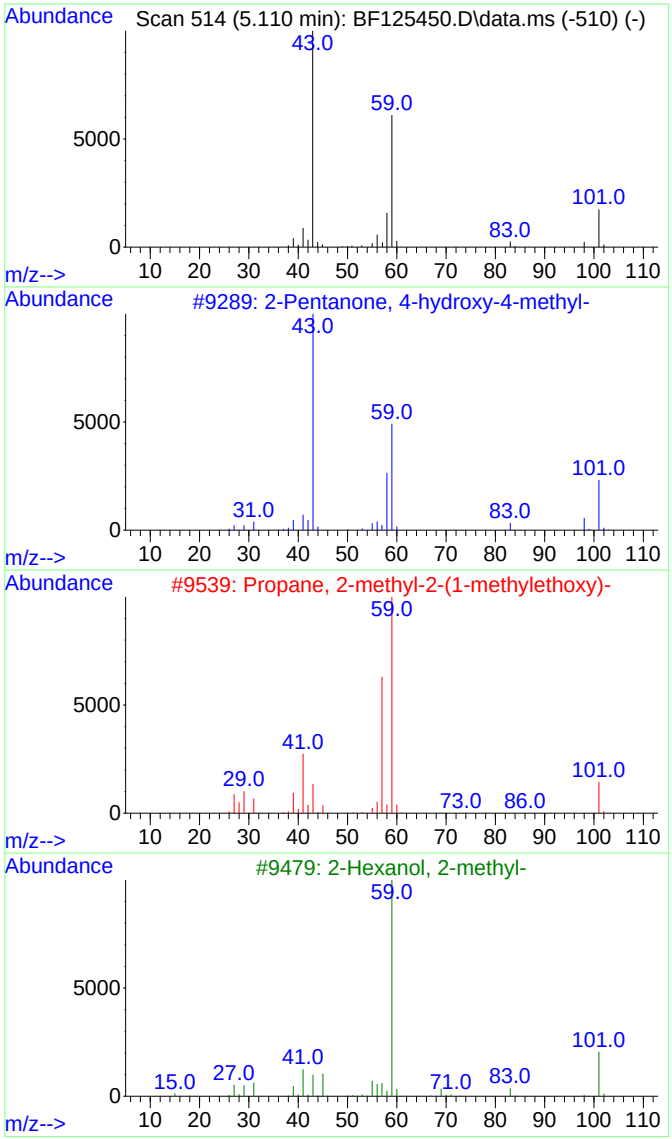
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

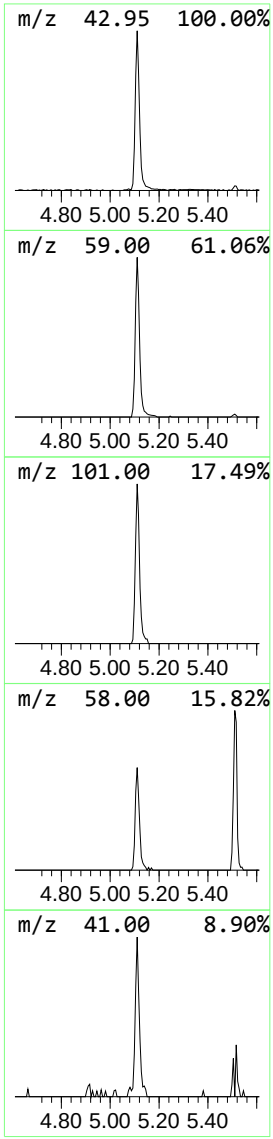
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.74 ng	265021	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	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	1,2-Butanediol	90	C4H10O2	000584-03-2	25





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Operator : JU/CG
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Misc :
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Instrument : BNA_F
ClientSampleId : A008015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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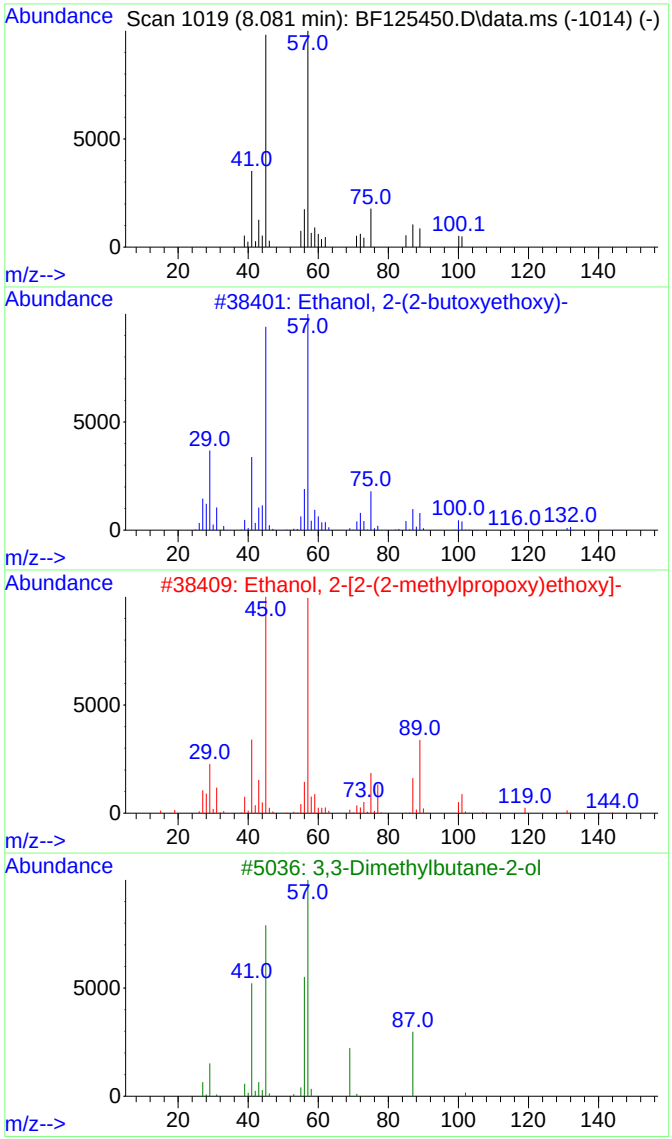
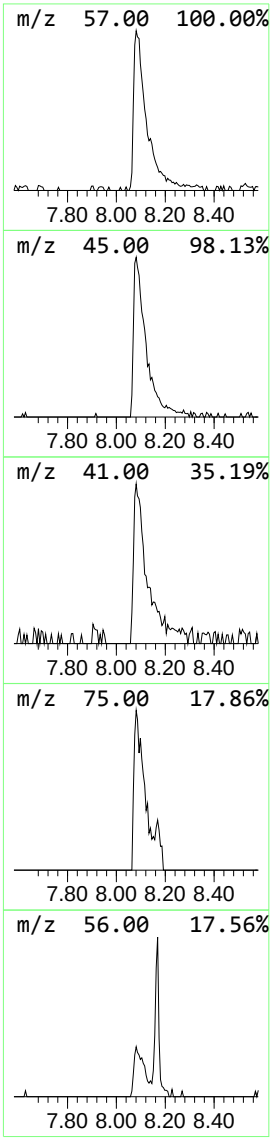
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	2.94 ng	185033	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	50





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Instrument : BNA_F
ClientSampleId : A008015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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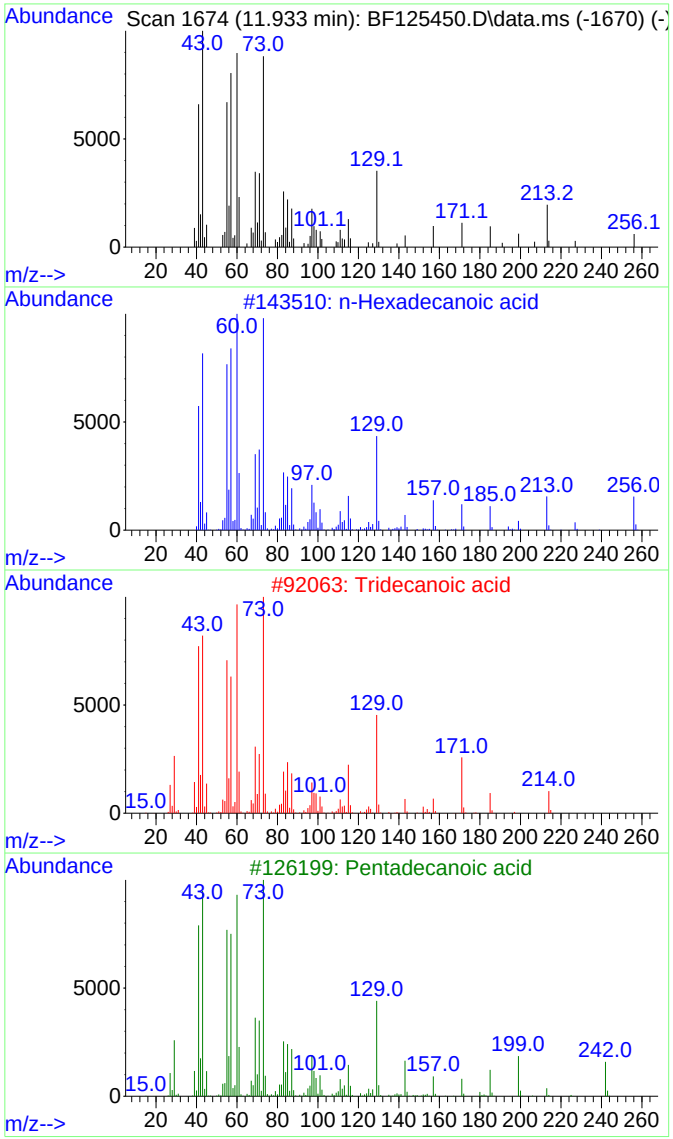
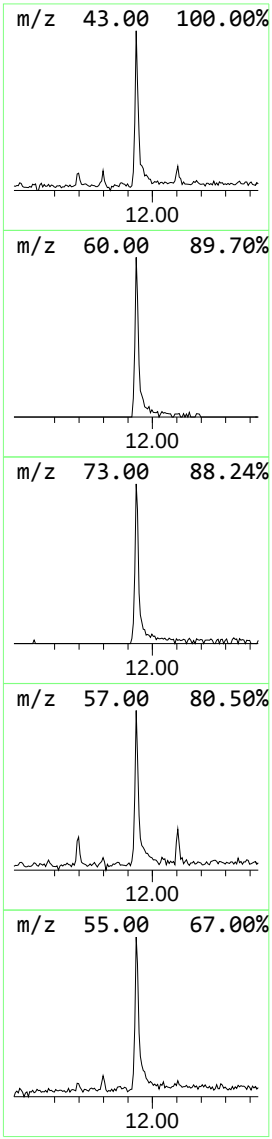
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.89 ng	210375	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Octanoic acid	144	C8H16O2	000124-07-2	47





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A008015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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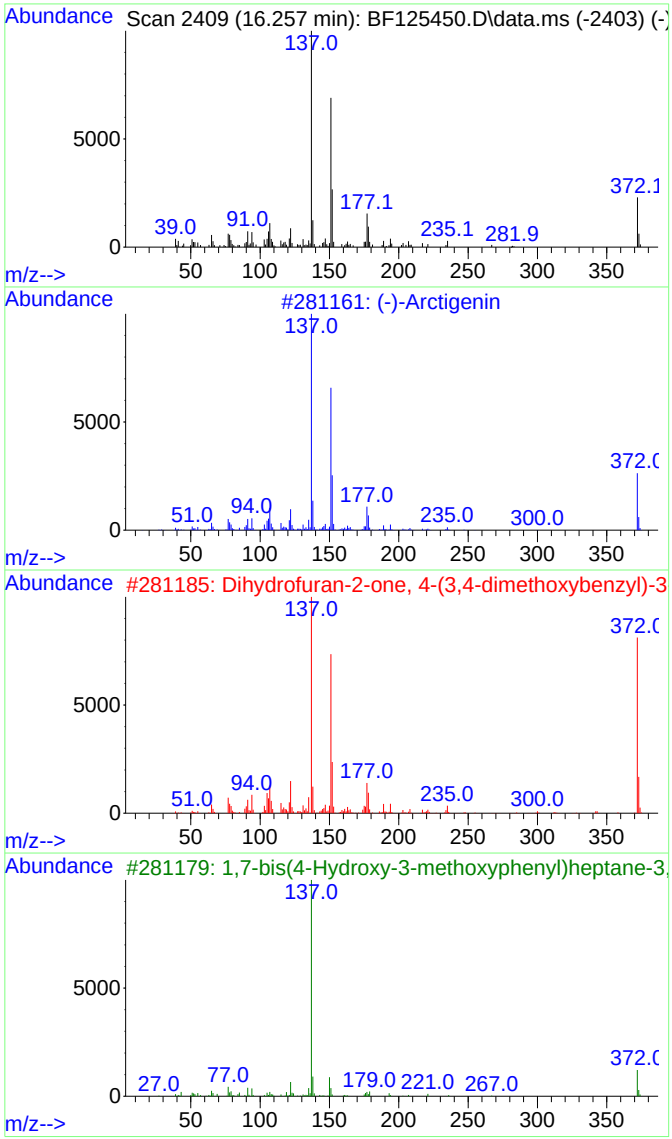
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

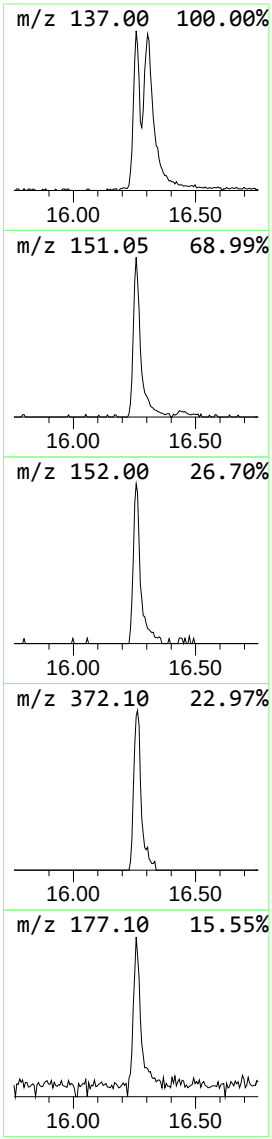
****

Peak Number 6 (-)-Arctigenin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	7.20 ng	327465	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Arctigenin	372	C21H24O6	007770-78-7	96
2	Dihydrofuran-2-one, 4-(3,4-dimet...	372	C21H24O6	026687-82-1	94
3	1,7-bis(4-Hydroxy-3-methoxypheny...	372	C21H24O6	036062-04-1	55
4	(-)-Nortrachelogenin	374	C20H22O7	034444-37-6	41
5	Phenol, 2-methoxy-4-(methoxymeth...	168	C9H12O3	005533-03-9	38





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TIC Library : C:\Database\NIST20.L
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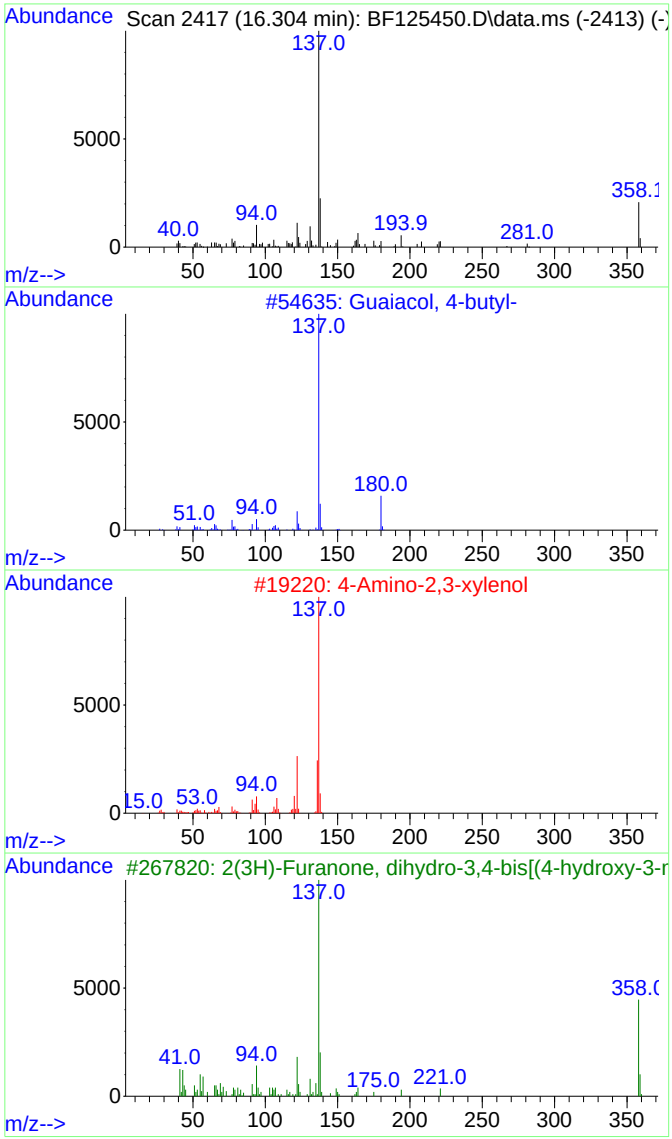
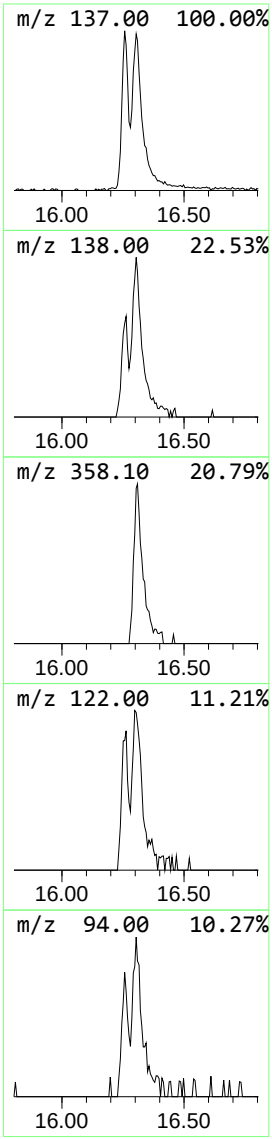
****

Peak Number 7 unknown16.304 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.304	6.25 ng	284206	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guaiacol, 4-butyl-	180	C11H16O2	059832-96-1	47
2	4-Amino-2,3-xylenol	137	C8H11NO	003096-69-3	47
3	2(3H)-Furanone, dihydro-3,4-bis[...	358	C20H22O6	000580-72-3	46
4	Phenol, 3-(cyclopentylaminomethy...	221	C13H19NO2	332382-83-9	40
5	3-(3-Hydroxy-4-methoxyphenyl)-l-...	211	C10H13NO4	1000103-80-4	40





Tentatively Identified Compound (LSC) summary

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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...	2.193	35.6	ng	1641620	1	6.887	922797	20.0
2-Pentanone, 4-...	5.110	5.7	ng	265021	1	6.887	922797	20.0
Ethanol, 2-(2-b...	8.081	2.9	ng	185033	2	8.169	1258830	20.0
n-Hexadecanoic ...	11.933	2.9	ng	210375	4	11.416	1456480	20.0
(-)-Arctigenin	16.257	7.2	ng	327465	6	15.557	909700	20.0
unknown16.304	16.304	6.3	ng	284206	6	15.557	909700	20.0