LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090421\
Data File : BF125378.D
Acq On : 4 Sep 2021 19:56
Operator : JU/CG
Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

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: BF125378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	12	22	28	rVB	2898836	4183616	100.00%	17.765%
2	3.898	301	308	315	rBV	68591	111514	2.67%	0.474%
3	5.116	511	515	522	rVB	175055	181236	4.33%	0.770%
4	5.522	581	584	597	rBV	1508512	1502252	35.91%	6.379%
5	6.528	751	755	764	rBV	820187	878966	21.01%	3.732%
6	6.898	814	818	821	rBV	898014	743291	17.77%	3.156%
7	7.304	882	887	893	rBV	61561	91751	2.19%	0.390%
8	7.457	909	913	916	rBV	2038446	1944707	46.48%	8.258%
9	7.781	965	968	973	rVB	58311	56062	1.34%	0.238%
10	7.892	984	987	990	rBV	55533	52770	1.26%	0.224%
11	8.086	1017	1020	1027	rBV2	79504	140374	3.36%	0.596%
12	8.181	1032	1036	1042	rVV	933347	837265	20.01%	3.555%
13	8.298	1042	1056	1060	rVV5	108440	250418	5.99%	1.063%
14	8.369	1064	1068	1070	rVB2	88709	94602	2.26%	0.402%
15	8.551	1093	1099	1101	rBV	184355	242321	5.79%	1.029%
16	8.598	1105	1107	1112	rVB2	114329	88879	2.12%	0.377%
17	8.798	1137	1141	1144	rBV2	92577	123247	2.95%	0.523%
18	9.257	1214	1219	1222	rBV	3464635	3172846	75.84%	13.473%
19	9.369	1235	1238	1242	rBV2	69926	72107	1.72%	0.306%
20	9.475	1253	1256	1259	rVB2	96110	85193	2.04%	0.362%
21	9.580	1271	1274	1276	rBV	65078	79094	1.89%	0.336%
22	9.686	1288	1292	1294	rBV2	204728	207872	4.97%	0.883%
23	9.745	1300	1302	1305	rVB2	91322	77444	1.85%	0.329%
24	9.933	1329	1334	1338	rBV	1027654	963057	23.02%	4.089%
25	10.727	1465	1469	1472	rBV	1972834	1751500	41.87%	7.437%
26	11.427	1585	1588	1590	rBV	744981	675714	16.15%	2.869%
27	11.451	1590	1592	1595	rVB	362536	256338	6.13%	1.088%
28	11.963	1677	1679	1681	rVB	325699	238195	5.69%	1.011%
29	13.015	1855	1858	1861	rBV	3122586	2726038	65.16%	11.575%
30	14.074	2035	2038	2042	rVB	860236	738827	17.66%	3.137%
31	15.574	2288	2293	2298	rVB	764660	982689	23.49%	4.173%

Sum of corrected areas: 23550185

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Misc :
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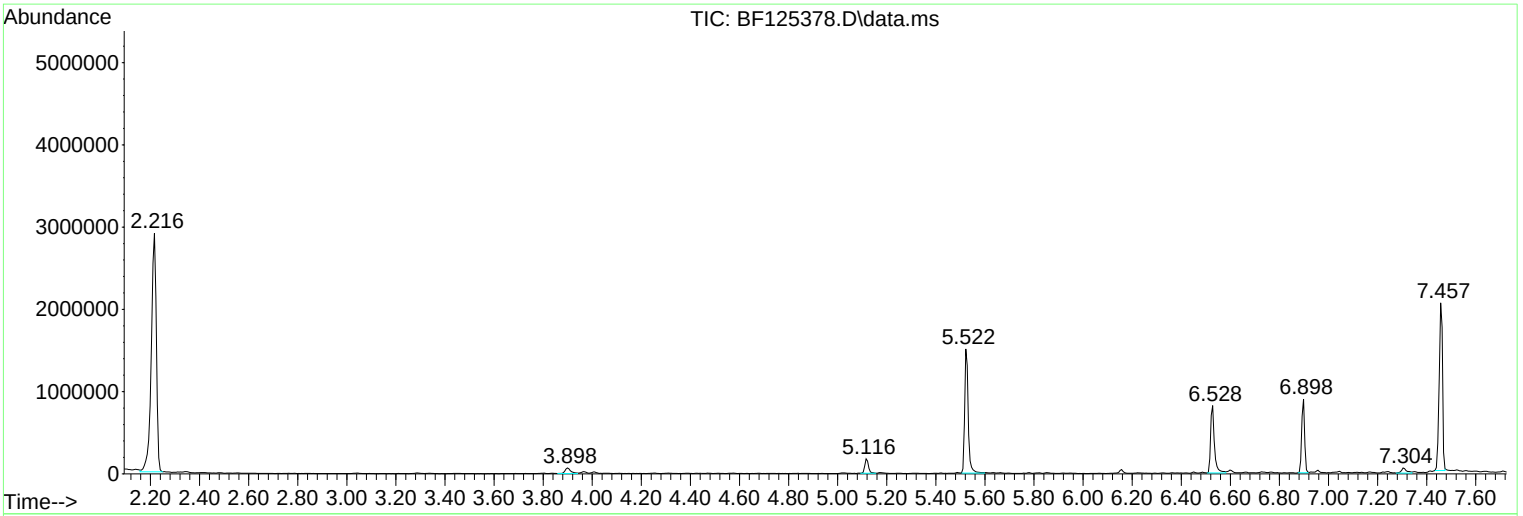
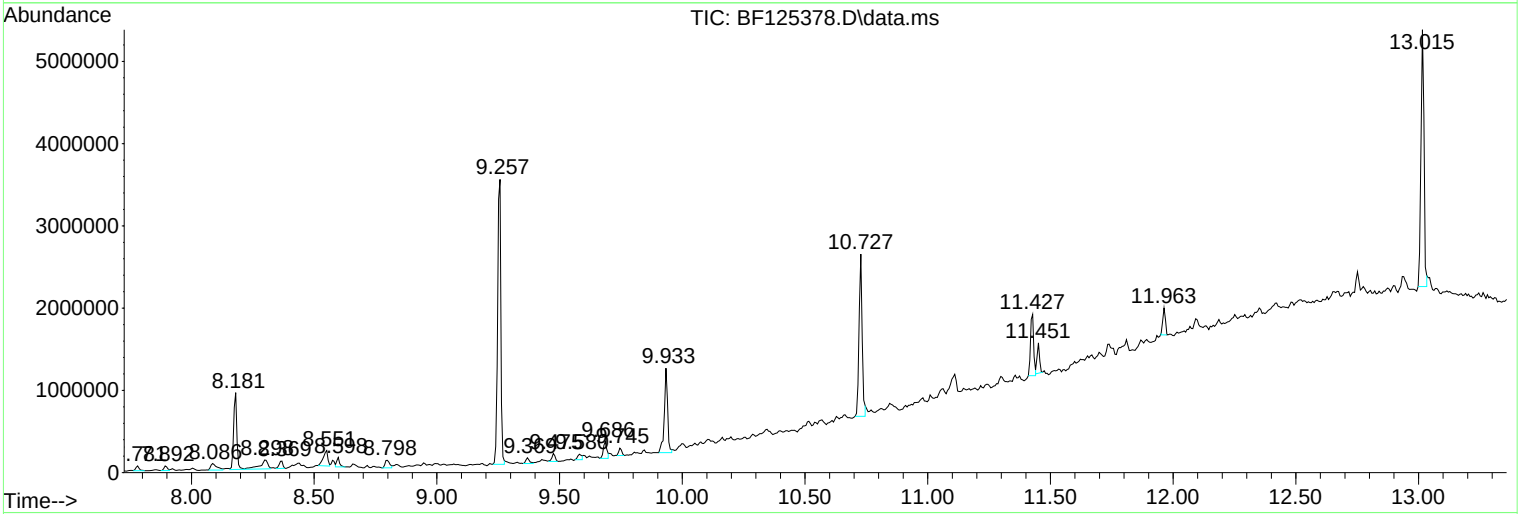
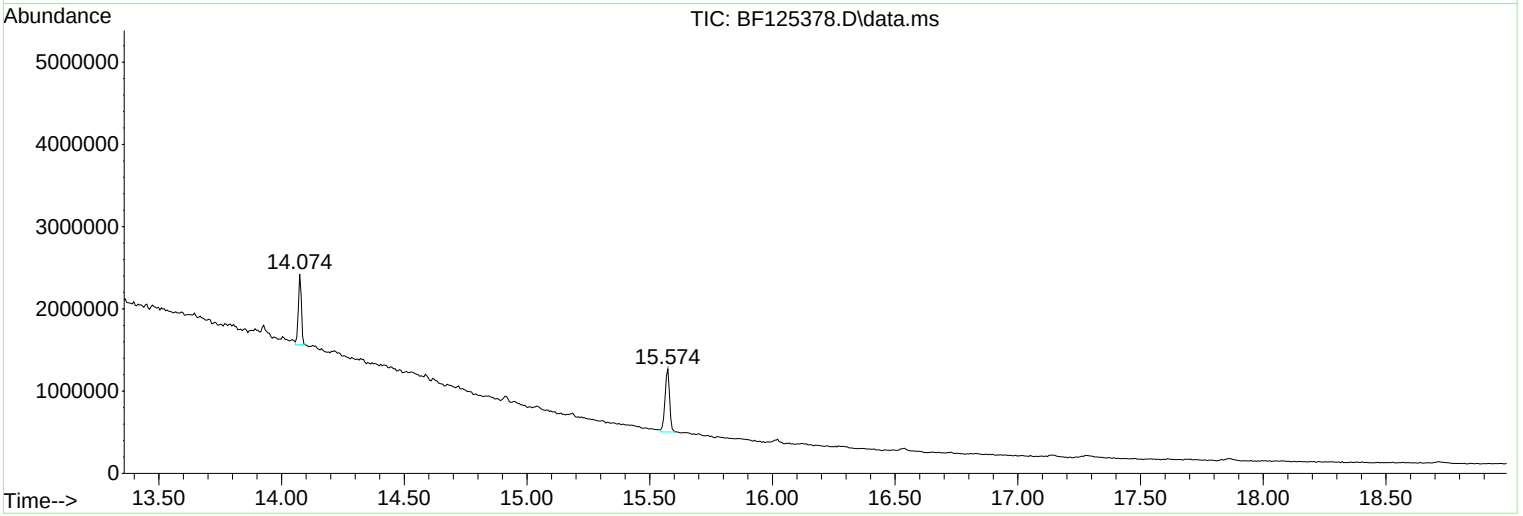
Instrument :
BNA_F
ClientSampleId :
93-94

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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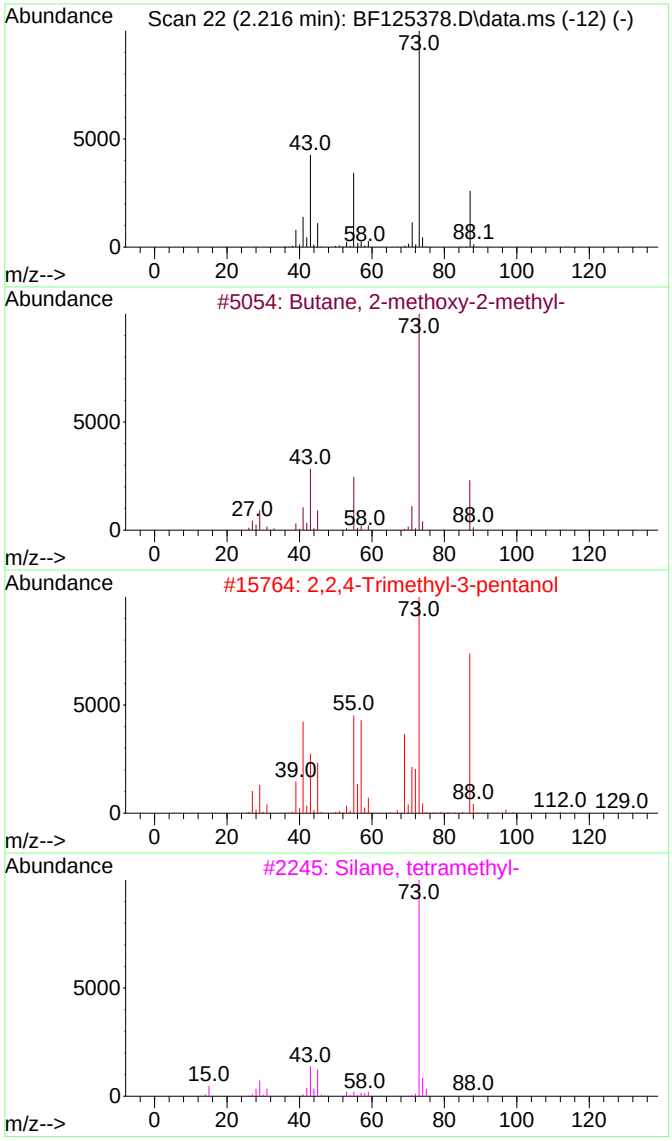
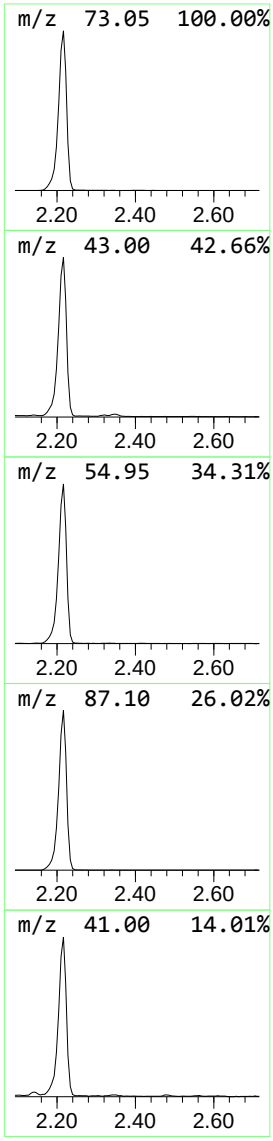
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	112.57 ng	4183620	1,4-Dichlorobenzene-d4	6.898

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Data File : BF125378.D
Acq On : 4 Sep 2021 19:56
Operator : JU/CG
Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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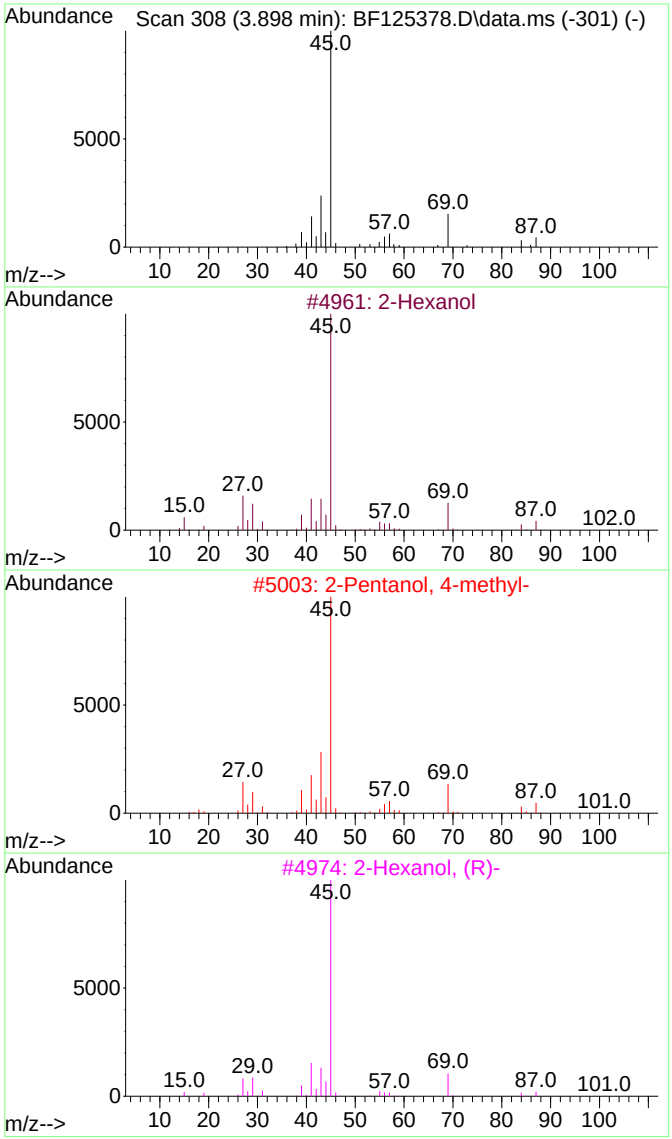
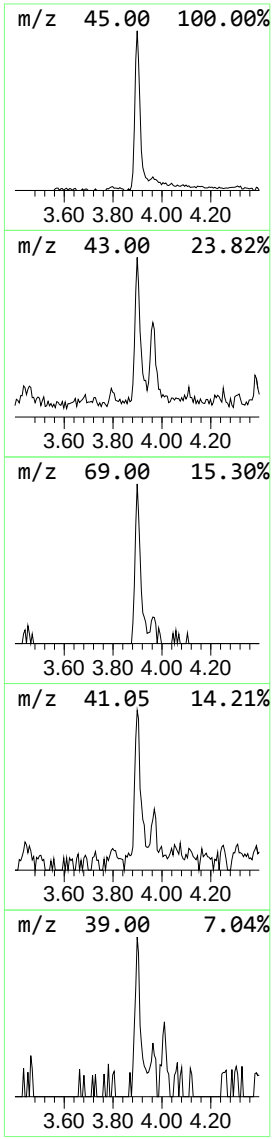
Peak Number 2 2-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.898	3.00 ng	111514	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol	102	C6H14O	000626-93-7	83
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3	2-Hexanol, (R)-	102	C6H14O	026549-24-6	83
4	2-Hexanol, (S)-	102	C6H14O	052019-78-0	64
5	2-Heptanol	116	C7H16O	000543-49-7	40





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Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

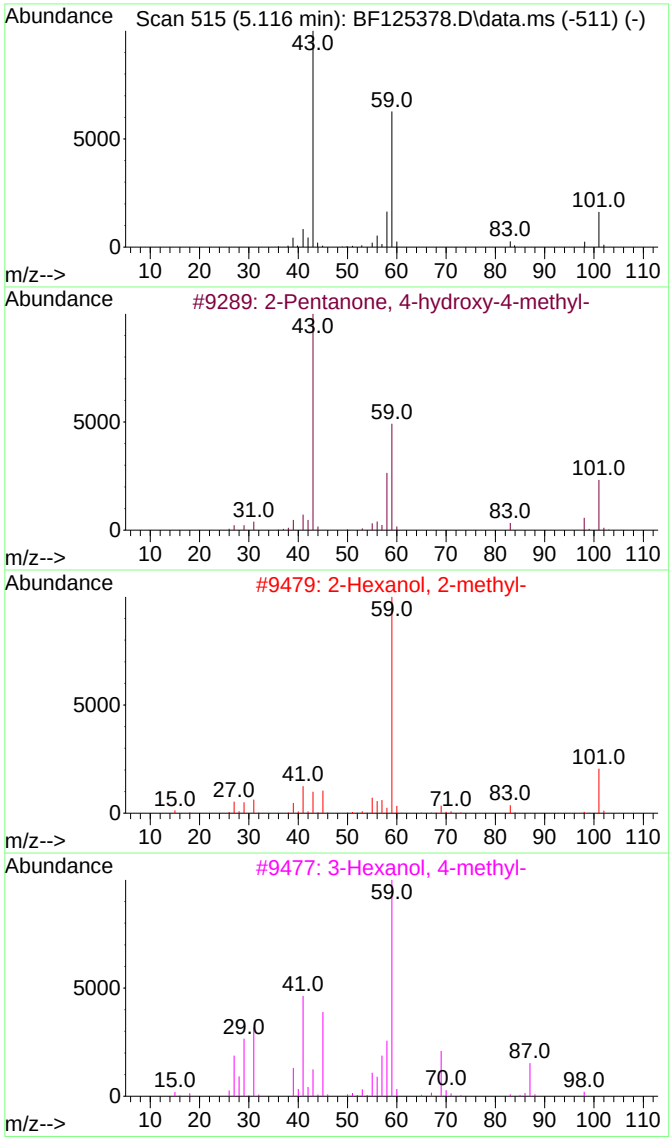
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

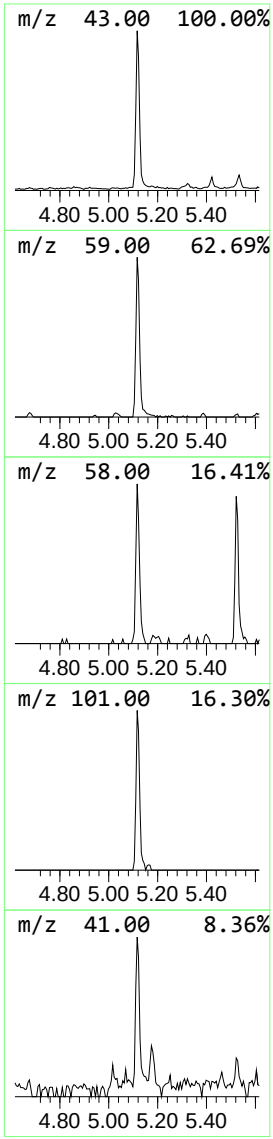
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	4.88 ng	181236	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Instrument : BNA_F
ClientSampleId : 93-94

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
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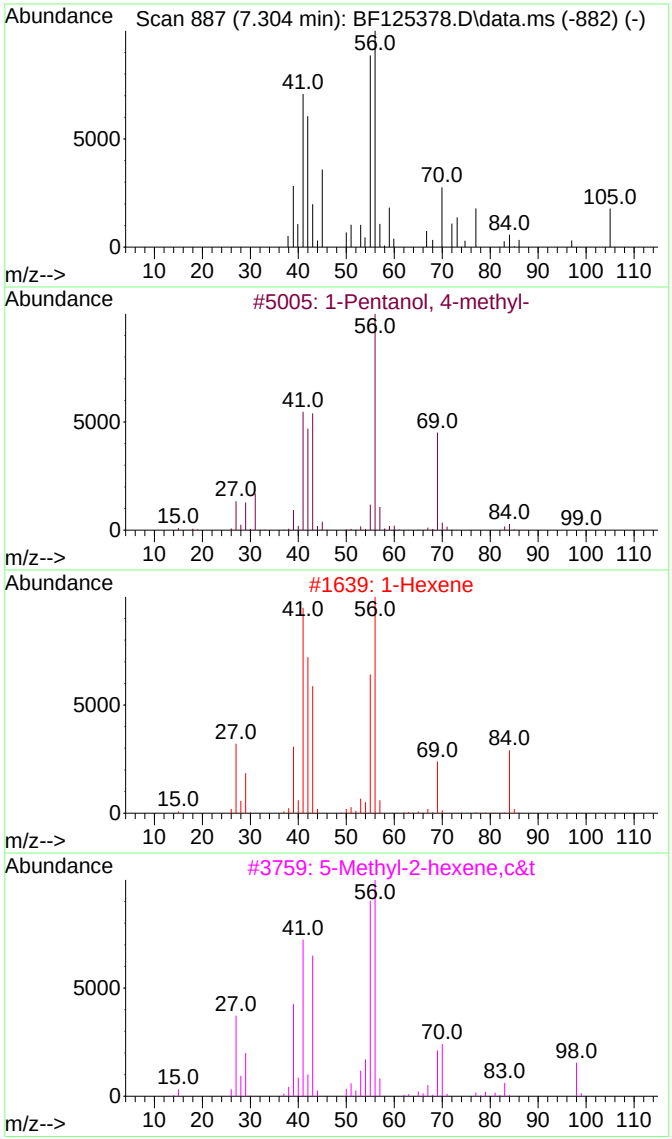
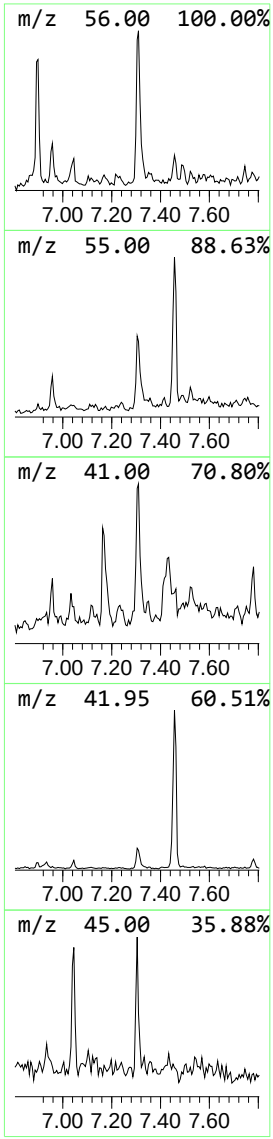
Peak Number 4 unknown7.304 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.304	2.47 ng	91751	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	47
2	1-Hexene	84	C6H12	000592-41-6	47
3	5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	43
4	(Z)-2-Heptene	98	C7H14	006443-92-1	38
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	38





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Operator : JU/CG
Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

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

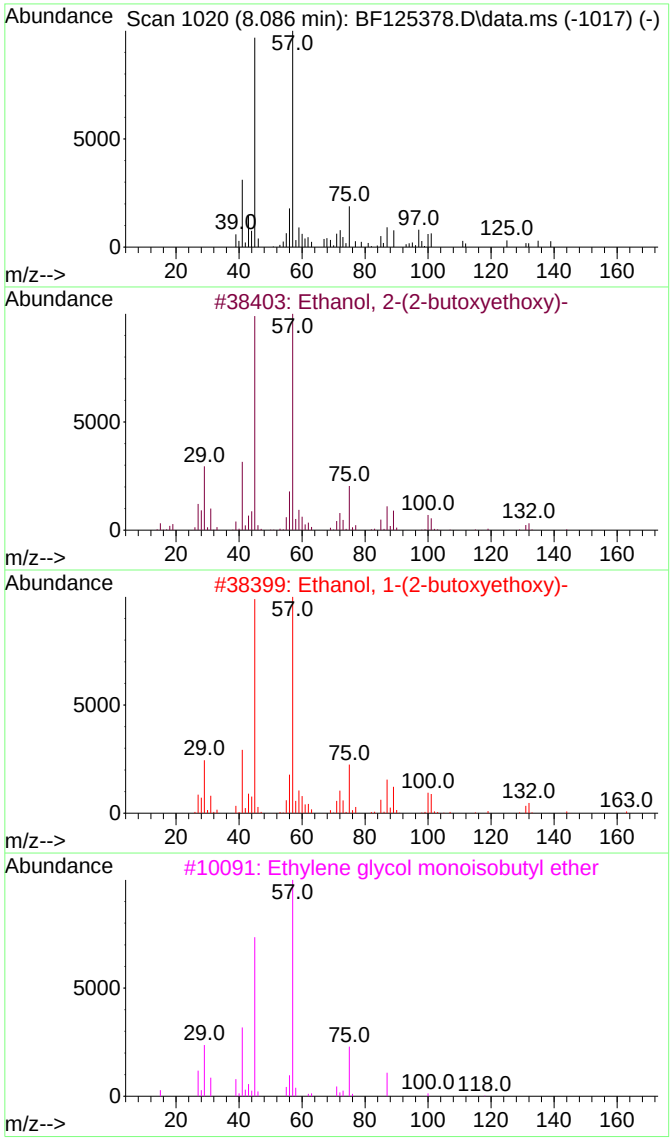
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

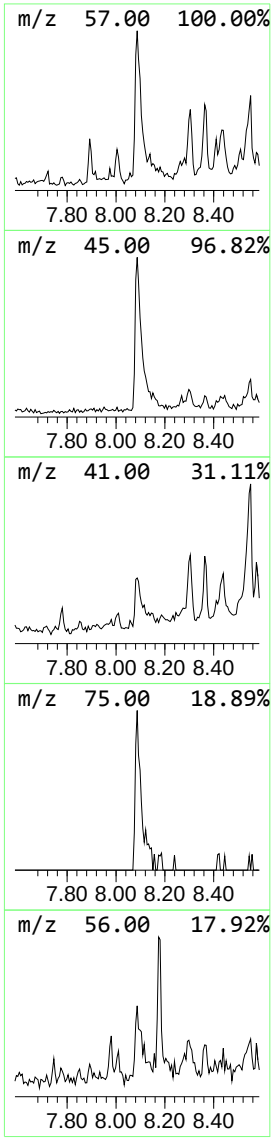
****

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.086	3.35 ng	140374	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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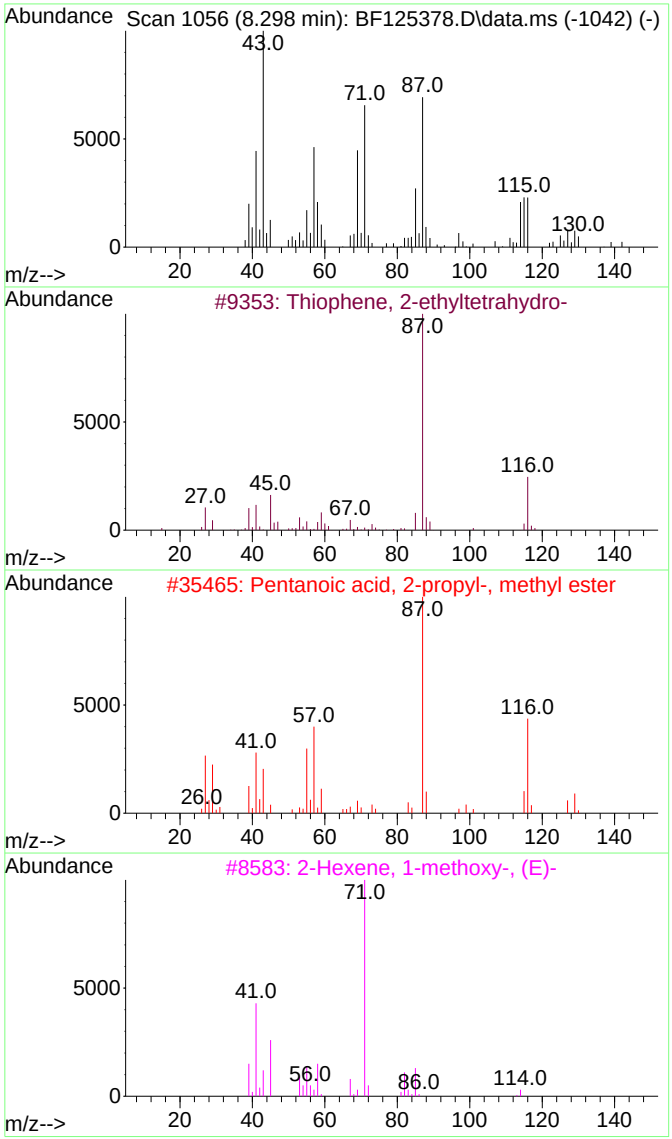
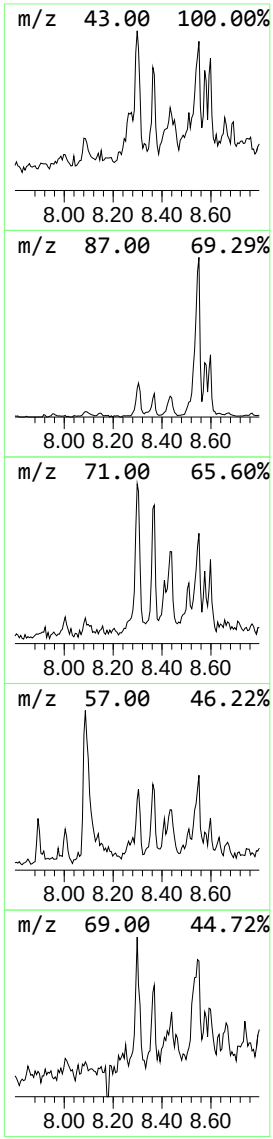
****

Peak Number 6 unknown8.298 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	5.98 ng	250418	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	30
2	Pentanoic acid, 2-propyl-, methy...	158	C9H18O2	022632-59-3	27
3	2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	27
4	1-Methoxycyclohexane	114	C7H14O	000931-56-6	22
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	14





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Instrument : BNA_F
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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
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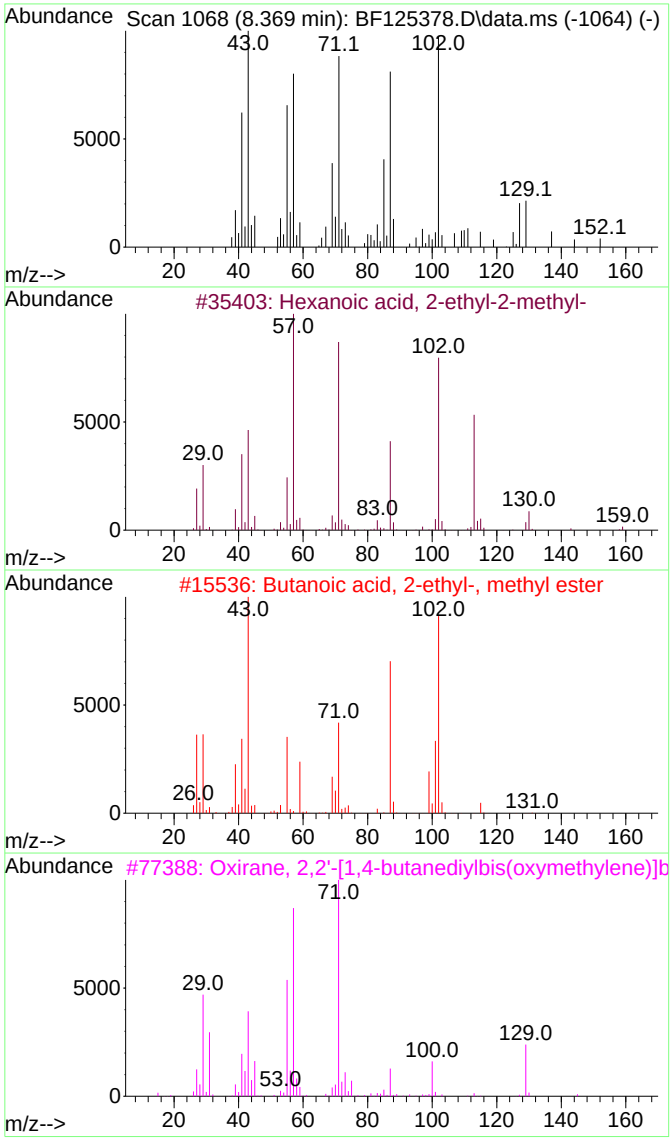
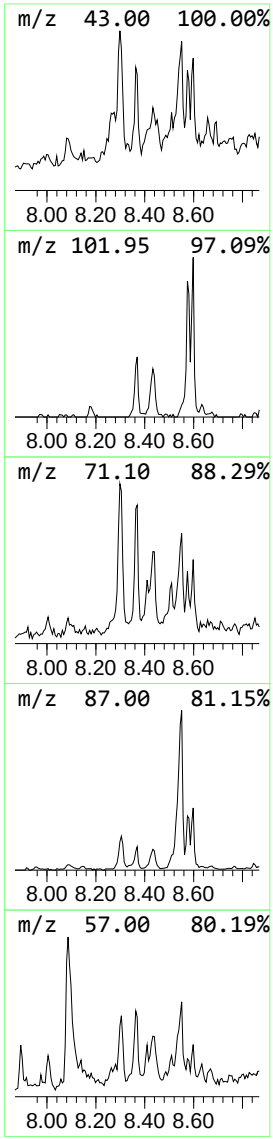
****

Peak Number 7 unknown8.369 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.369	2.26 ng	94602	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-2-methyl-	158	C9H18O2	001185-29-1	47
2	Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	43
3	Oxirane, 2,2'-[1,4-butanediylbis...	202	C10H18O4	002425-79-8	27
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	22
5	Sulfurous acid, decyl pentyl ester	292	C15H32O3S	1000309-14-3	22





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TIC Library : C:\Database\NIST20.L
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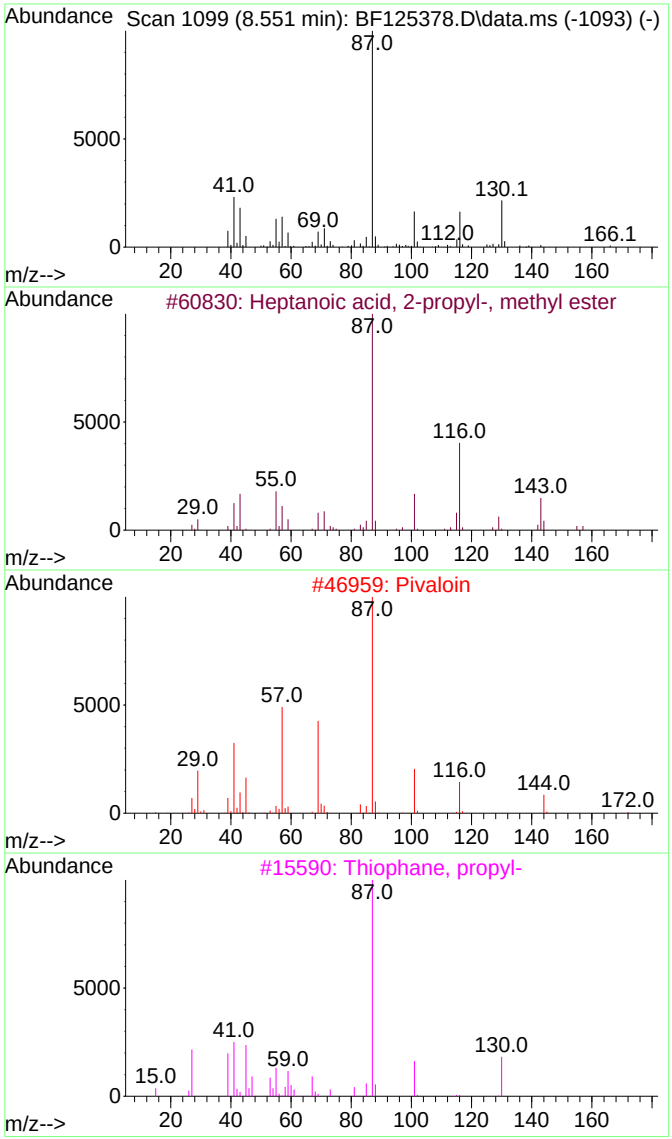
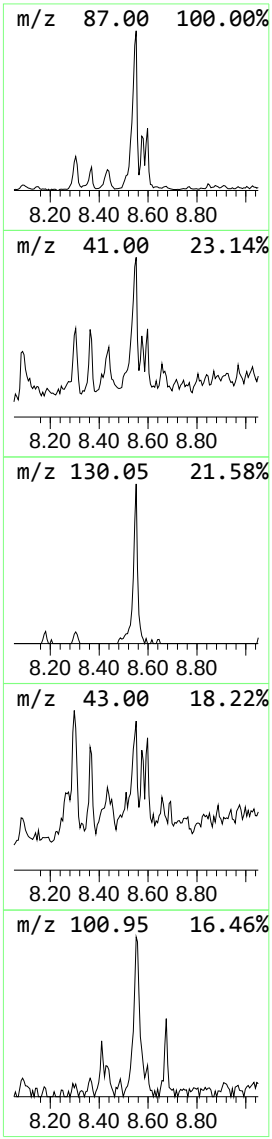
****
Peak Number 8 Heptanoic acid, 2-propyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	5.79 ng	242321	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	72
2	Pivaloin	172	C10H20O2	000815-66-7	64
3	Thiophane, propyl-	130	C7H14S	001551-34-4	64
4	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	59
5	1,3-Dioxane	88	C4H8O2	000505-22-6	47





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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

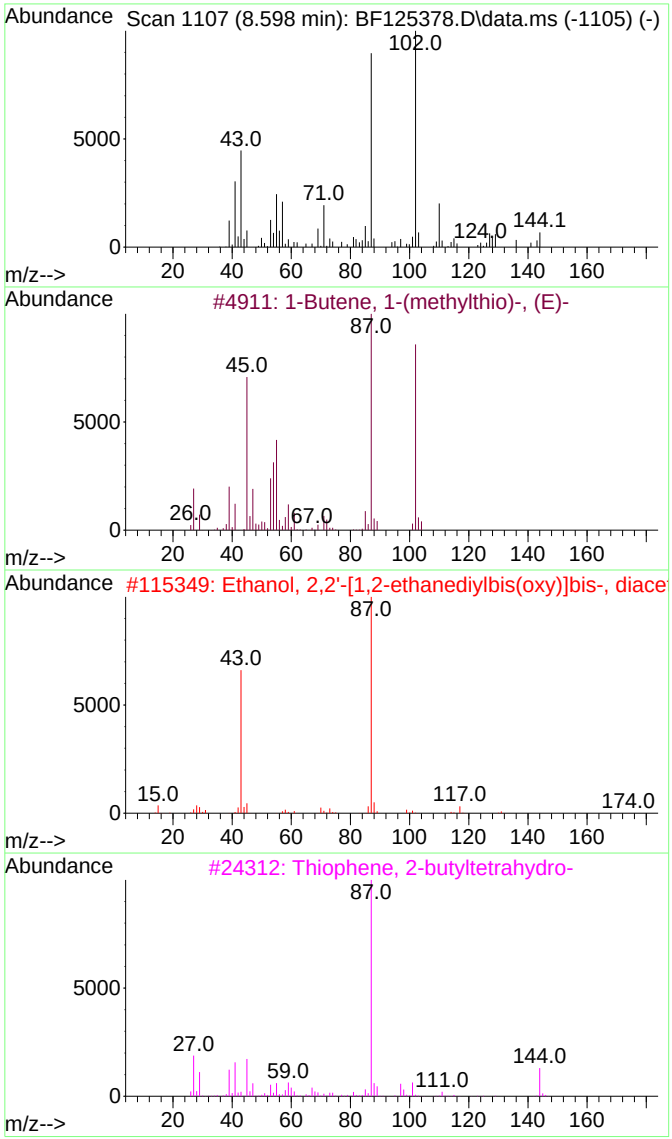
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

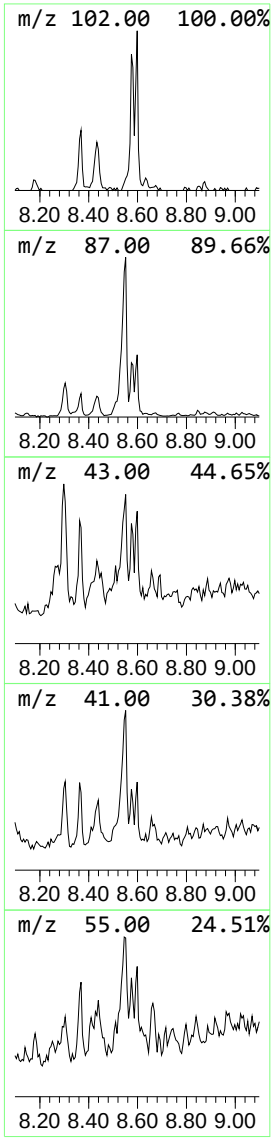
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Butene, 1-(methylthio)-, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.598	2.12 ng	88879	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	53
2	Ethanol, 2,2'-[1,2-ethanediylbis...	234	C10H18O6	000111-21-7	22
3	Thiophene, 2-butyltetrahydro-	144	C8H16S	001613-49-6	22
4	Pentanamide, N-ethyl-	129	C7H15NO	054007-33-9	22
5	1,3-Dioxolane, 2-(1,1-dimethylet...	144	C8H16O2	006135-54-2	22





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Data File : BF125378.D
Acq On : 4 Sep 2021 19:56
Operator : JU/CG
Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

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

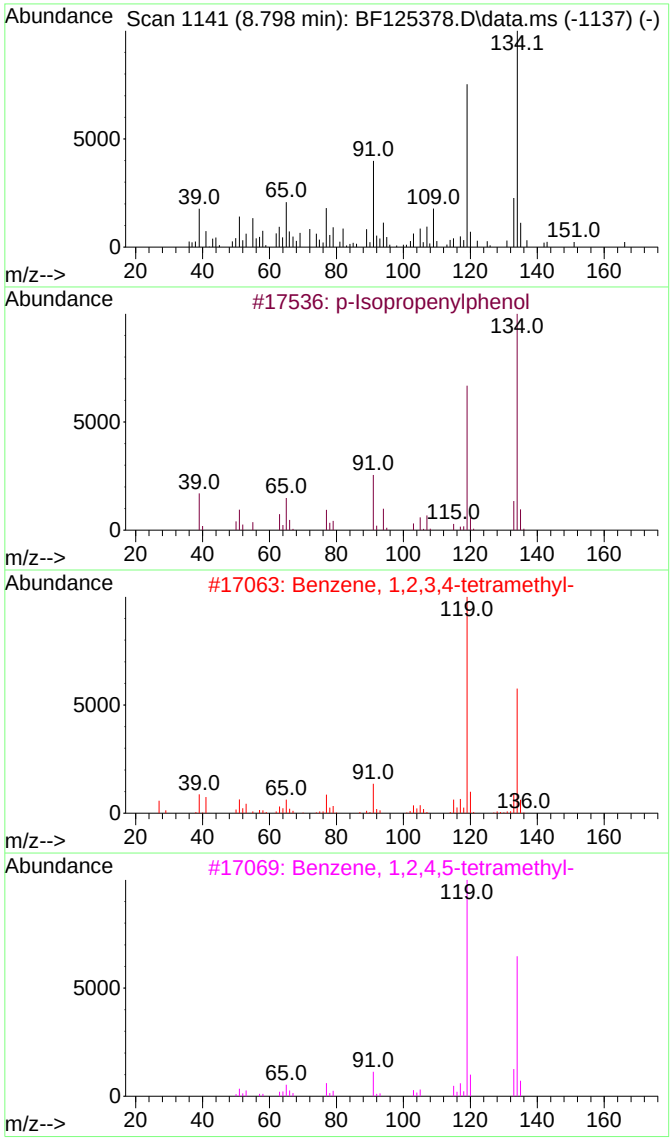
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

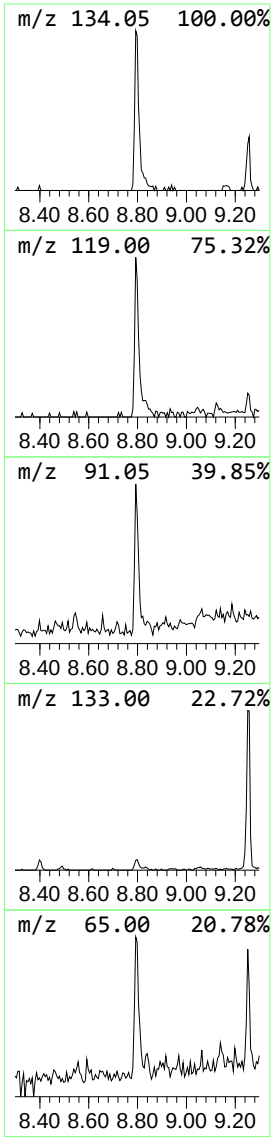
****

Peak Number 10 p-Isopropenylphenol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.798	2.94 ng	123247	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Isopropenylphenol	134	C9H10O	004286-23-1	93
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81





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Data File : BF125378.D
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Operator : JU/CG
Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

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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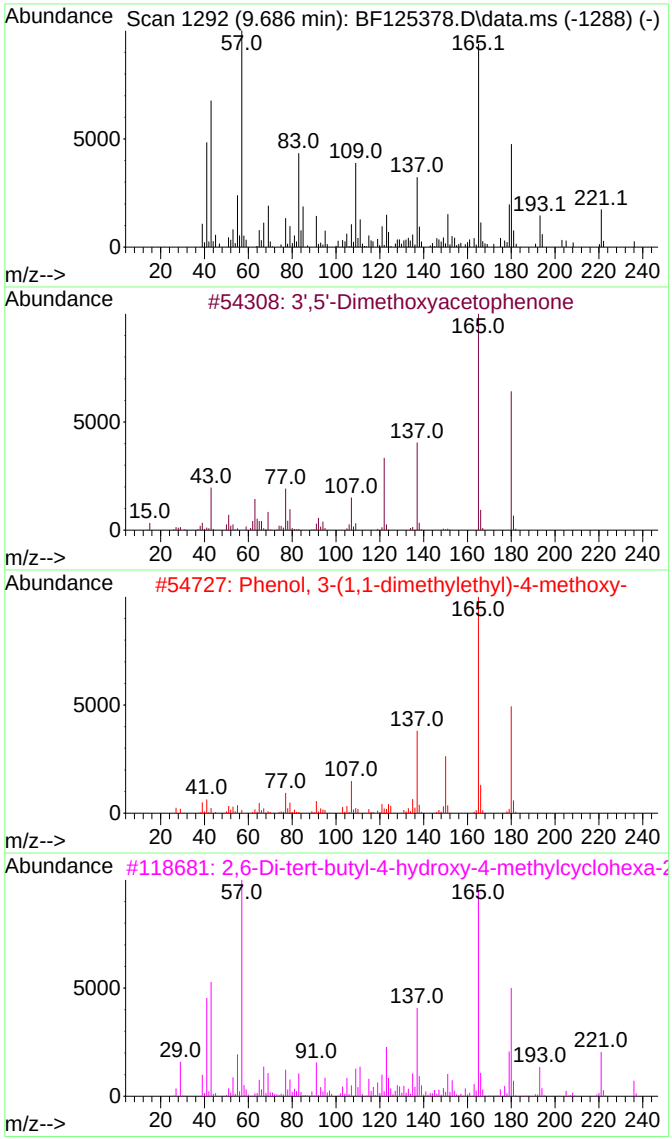
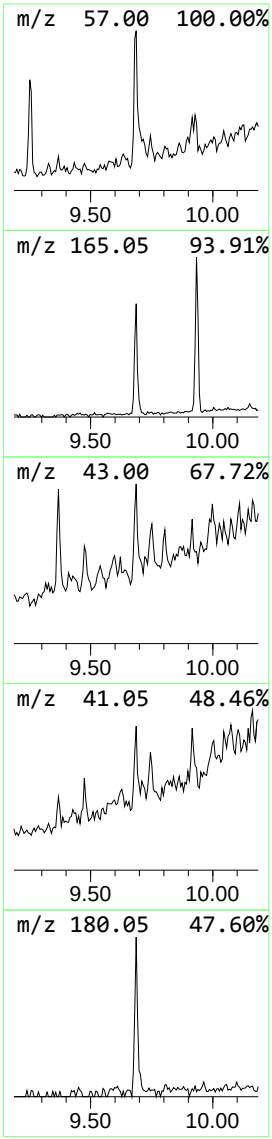
Peak Number 11 3',5'-Dimethoxyacetophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.686	4.32 ng	207872	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	55
2	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	55
3	2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	52
4	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	50
5	Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	001201-38-3	45





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Data File : BF125378.D
Acq On : 4 Sep 2021 19:56
Operator : JU/CG
Sample : M3646-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

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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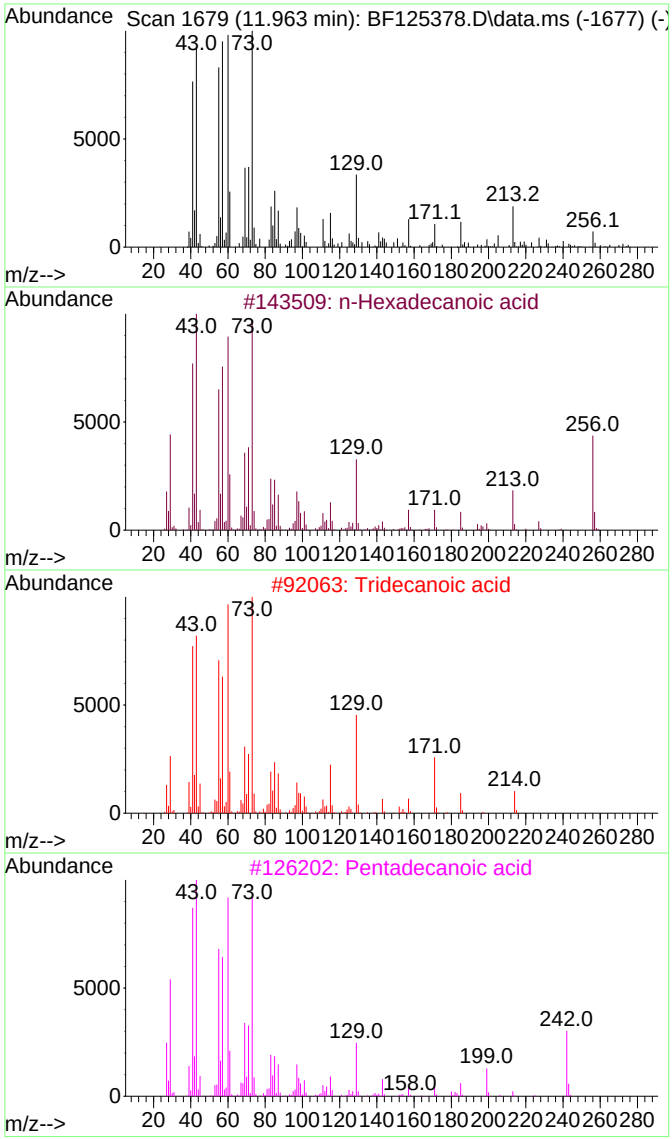
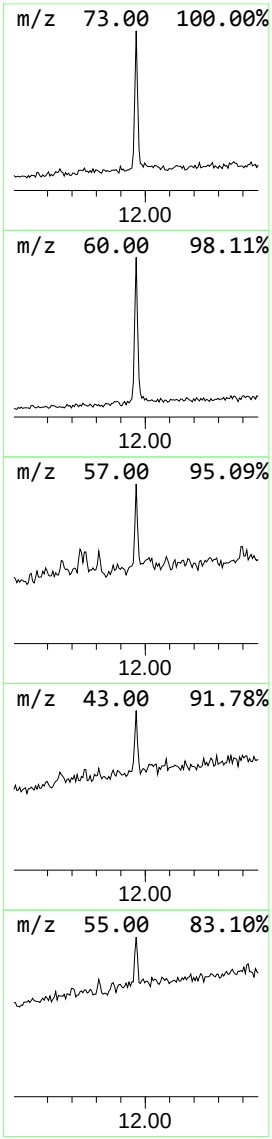
Peak Number 12 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	7.05 ng	238195	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Tentatively Identified Compound (LSC) summary

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Data File : BF125378.D
Acq On : 4 Sep 2021 19:56
Operator : JU/CG
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 93-94

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.216	112.6	ng	4183620	1	6.898	743291	20.0
2-Hexanol	3.898	3.0	ng	111514	1	6.898	743291	20.0
2-Pentanone, 4-...	5.116	4.9	ng	181236	1	6.898	743291	20.0
unknown7.304	7.304	2.5	ng	91751	1	6.898	743291	20.0
Ethanol, 2-(2-b...	8.086	3.4	ng	140374	2	8.181	837265	20.0
unknown8.298	8.298	6.0	ng	250418	2	8.181	837265	20.0
unknown8.369	8.369	2.3	ng	94602	2	8.181	837265	20.0
Heptanoic acid,...	8.551	5.8	ng	242321	2	8.181	837265	20.0
1-Butene, 1-(me...	8.598	2.1	ng	88879	2	8.181	837265	20.0
p-Isopropenylph...	8.798	2.9	ng	123247	2	8.181	837265	20.0
3',5'-Dimethoxy...	9.686	4.3	ng	207872	3	9.933	963057	20.0
n-Hexadecanoic ...	11.963	7.0	ng	238195	4	11.427	675714	20.0