LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080874.D
Acq On : 5 Aug 2015 10:39
Operator : TP/UM
Sample : G3127-19
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EAST-ABUT-1(0-2)

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:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.133	3	4	7	rVB	24768	36784	1.66%	0.210%
2	3.184	94	96	105	rBV	24488	64726	2.92%	0.370%
3	4.361	197	199	204	rVB	58577	87211	3.93%	0.499%
4	5.024	253	257	260	rBV	1086138	1853558	83.58%	10.605%
5	5.436	290	293	295	rBV	1917428	1958154	88.30%	11.203%
6	5.836	326	328	331	rVB	80274	67489	3.04%	0.386%
7	6.464	379	383	385	rBV	1718521	2217624	100.00%	12.688%
8	6.590	391	394	397	rBV	1634525	1860805	83.91%	10.646%
9	6.819	412	414	417	rBB	282873	376680	16.99%	2.155%
10	6.979	426	428	431	rBV	1452159	1397093	63.00%	7.993%
11	7.390	461	464	466	rBV	1267070	1417812	63.93%	8.112%
12	8.110	524	527	529	rVB	345124	442789	19.97%	2.533%
13	9.185	618	621	623	rBV	1915664	1894752	85.44%	10.840%
14	9.573	653	655	657	rBV	271120	220449	9.94%	1.261%
15	9.859	677	680	682	rVB	382318	410056	18.49%	2.346%
16	10.636	746	748	751	rBV2	761255	822969	37.11%	4.708%
17	10.762	758	759	764	rVB	28895	34627	1.56%	0.198%
18	11.208	797	798	800	rBV	22751	23340	1.05%	0.134%
19	11.333	807	809	811	rBV	423045	347512	15.67%	1.988%
20	12.122	876	878	880	rVB	73805	57196	2.58%	0.327%
21	12.751	931	933	935	rBV	52550	46861	2.11%	0.268%
22	12.922	945	948	950	rBV	893450	997615	44.99%	5.708%
23	13.448	992	994	997	rBV2	34053	39199	1.77%	0.224%
24	13.494	997	998	1003	rVB3	12005	22190	1.00%	0.127%
25	13.962	1036	1039	1041	rBV	379112	341984	15.42%	1.957%
26	15.368	1159	1162	1165	rBV	274589	403847	18.21%	2.311%
27	20.283	1585	1592	1597	rBV6	6804	35311	1.59%	0.202%

Sum of corrected areas: 17478633

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Instrument :
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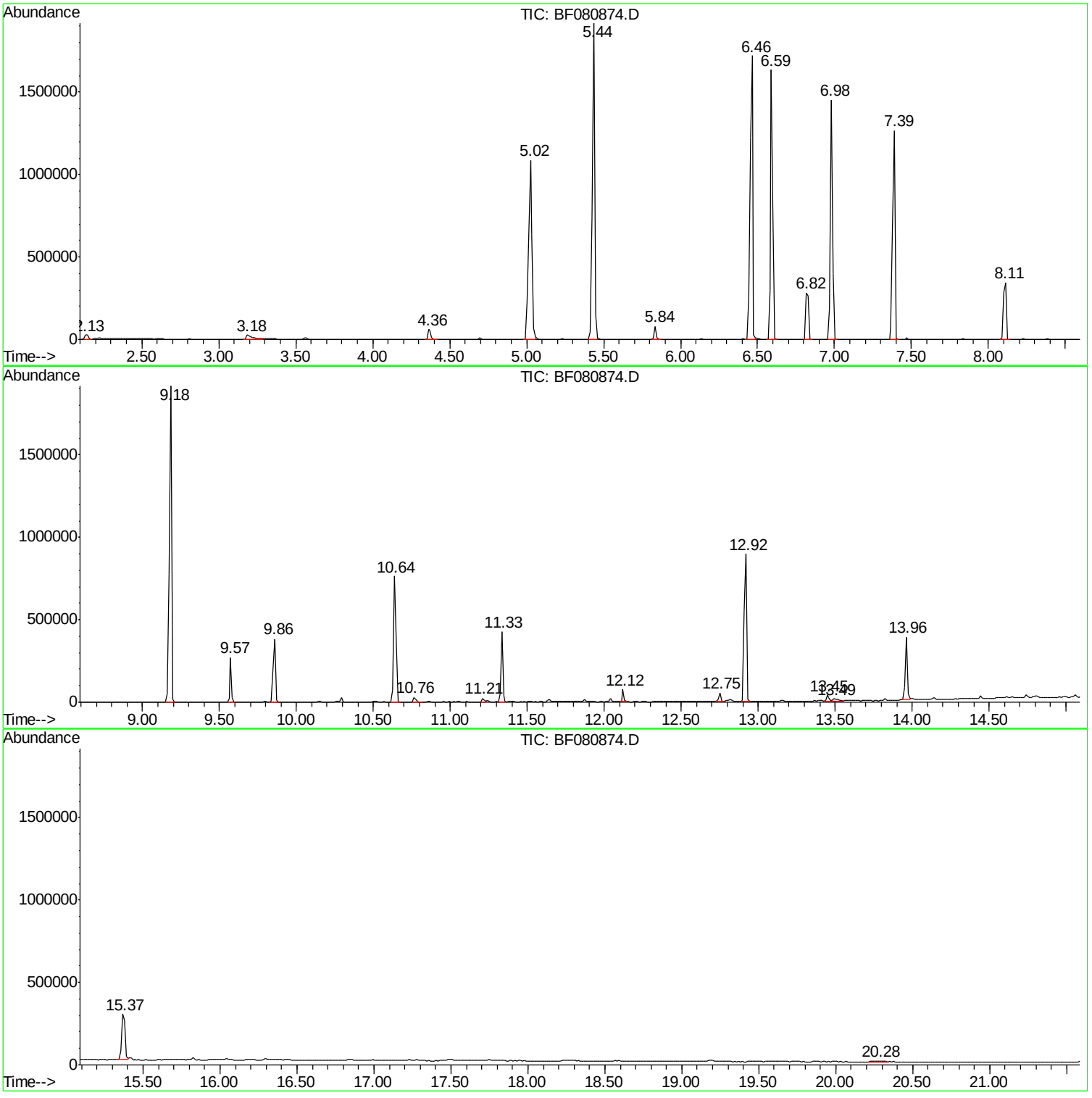
ClientSampleId :
EAST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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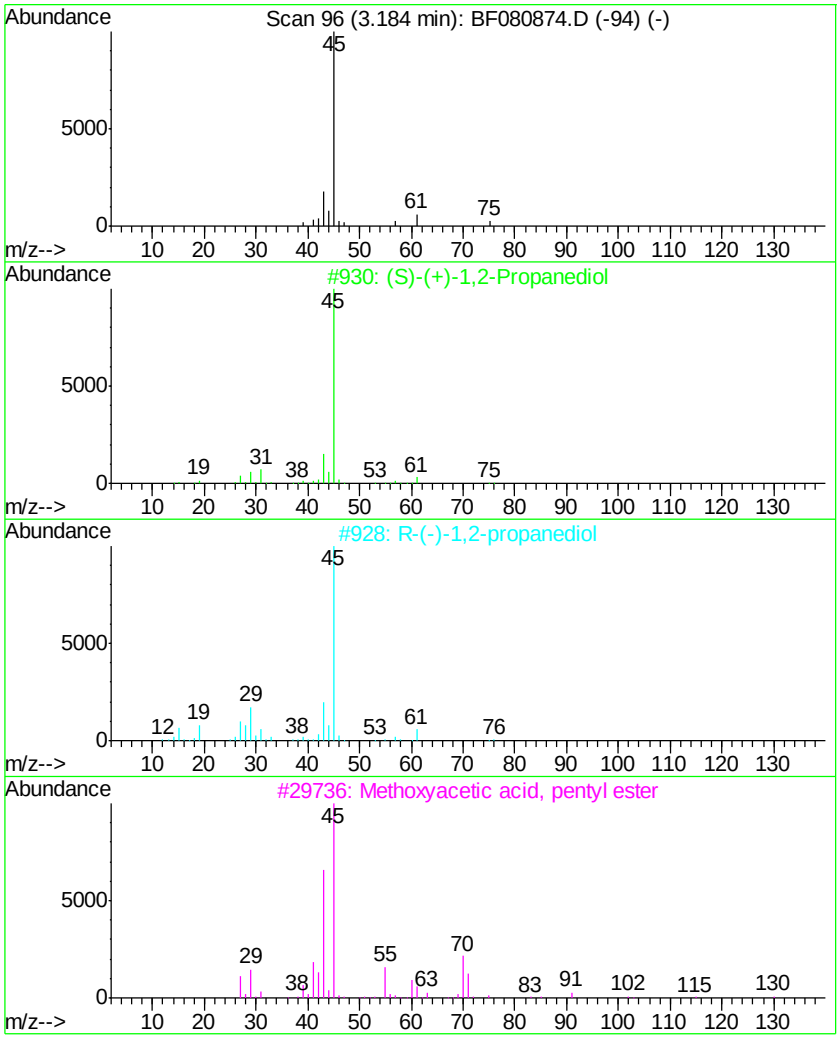
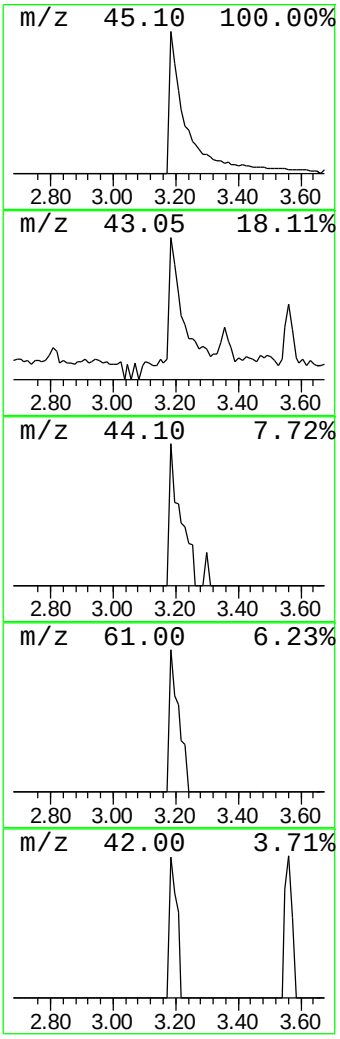
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	3.44 ng	64726	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9





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Instrument : BNA_F
ClientSampleId : EAST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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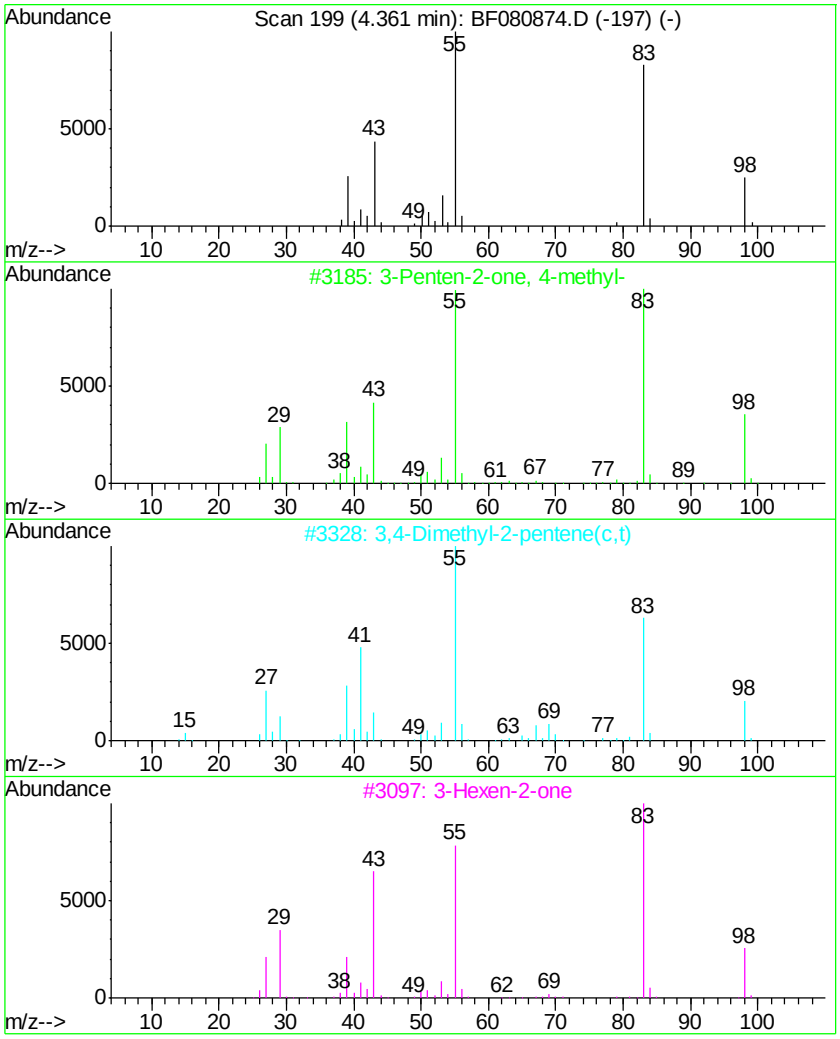
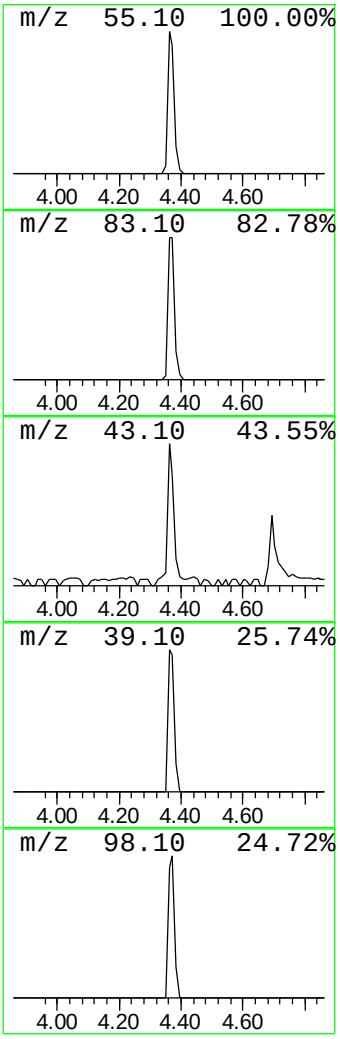
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	4.63 ng	87211	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3	3-Hexen-2-one	98	C6H10O	000763-93-9	80
4	Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	72
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72





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Instrument : BNA_F
ClientSampleId : EAST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
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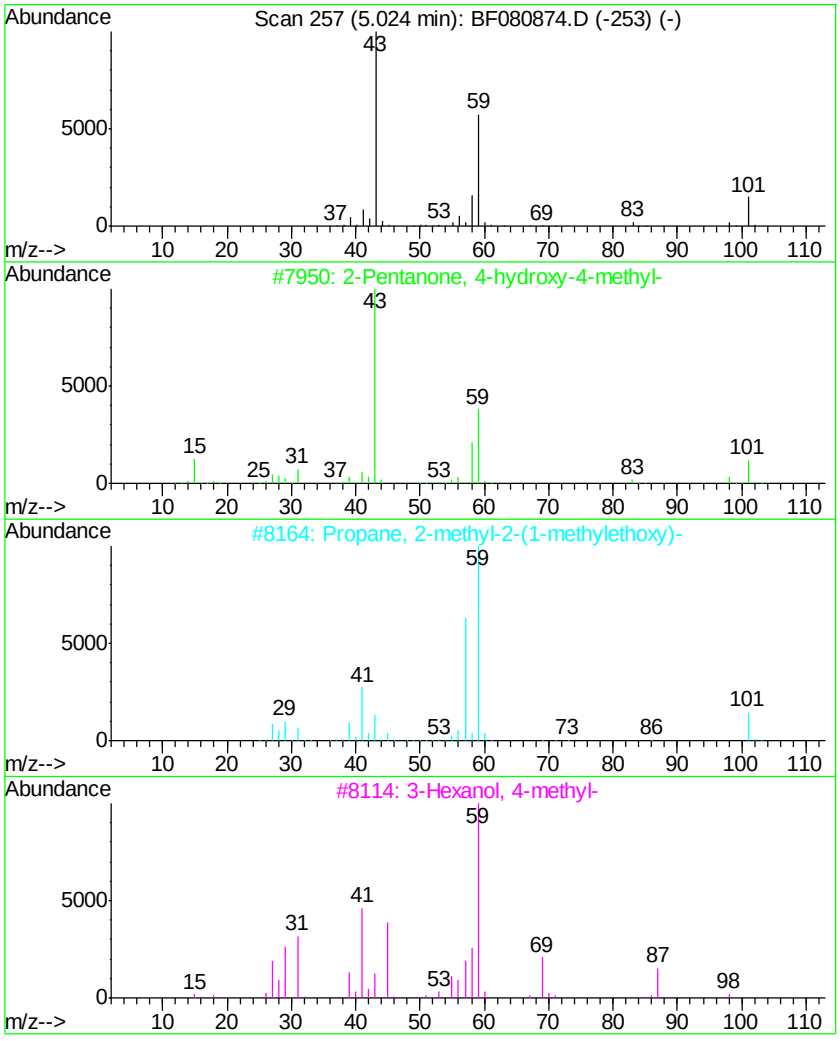
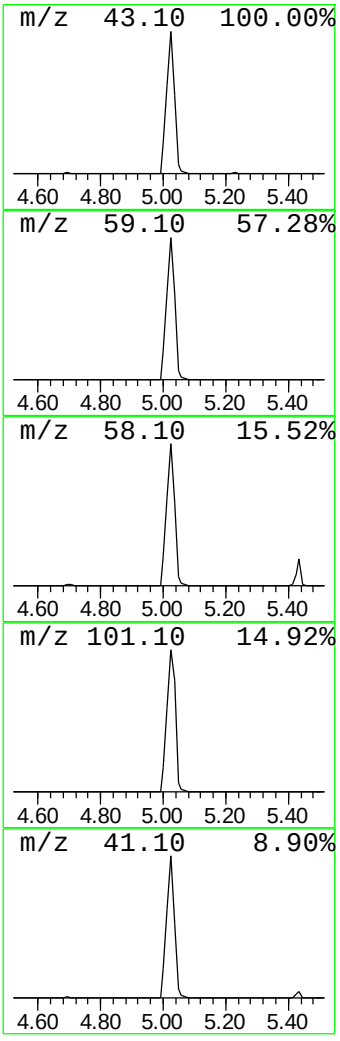
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	98.42 ng	1853560	1,4-Dichlorobenzene-d4	6.83

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	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : G3127-19
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EAST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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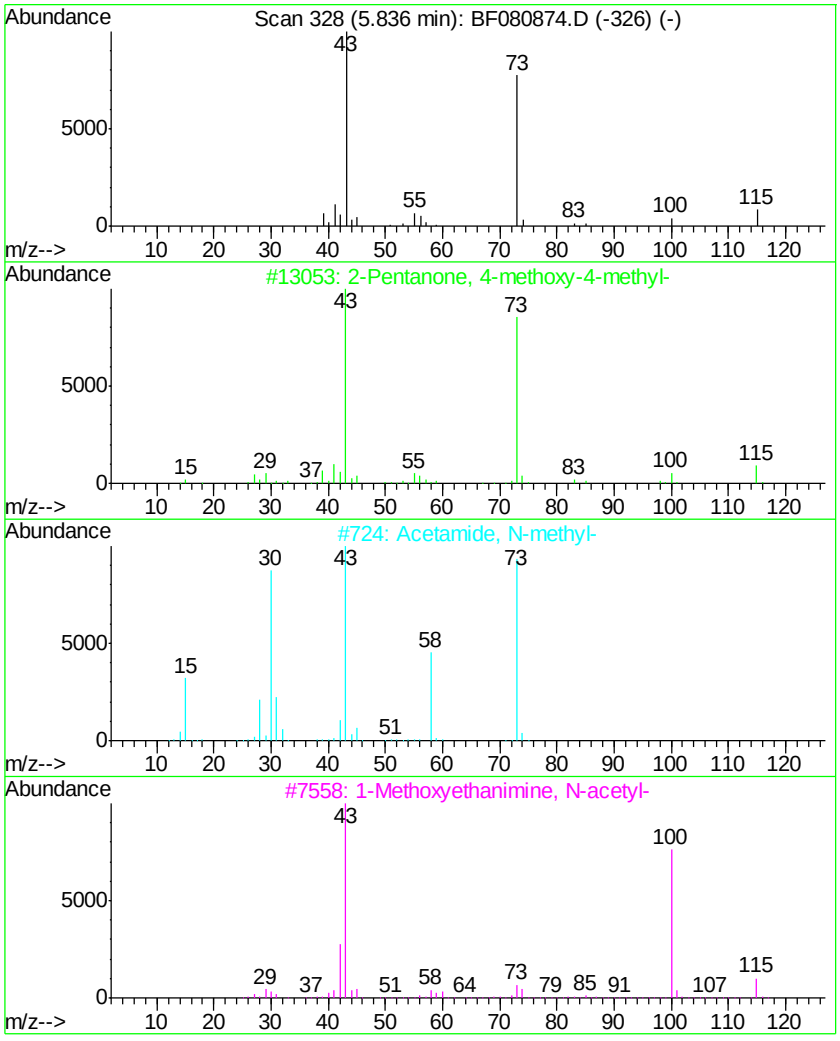
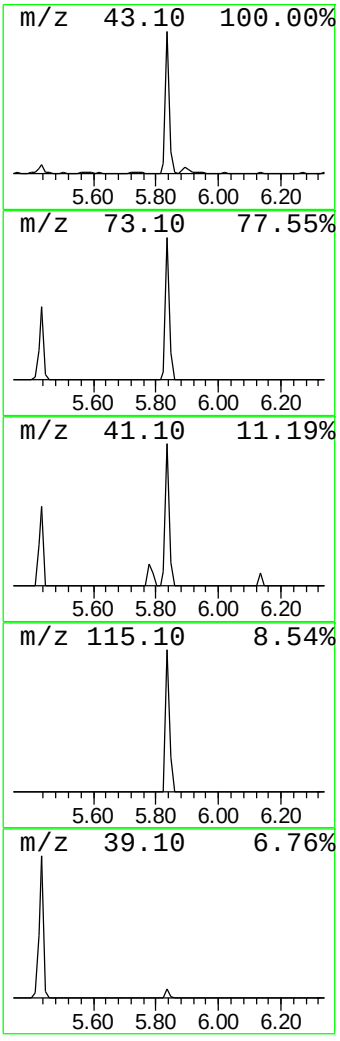
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.84	3.58 ng	67489	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	37
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
4	Hexane, 2-methyl-	100	C7H16	000591-76-4	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





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Sample : G3127-19
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
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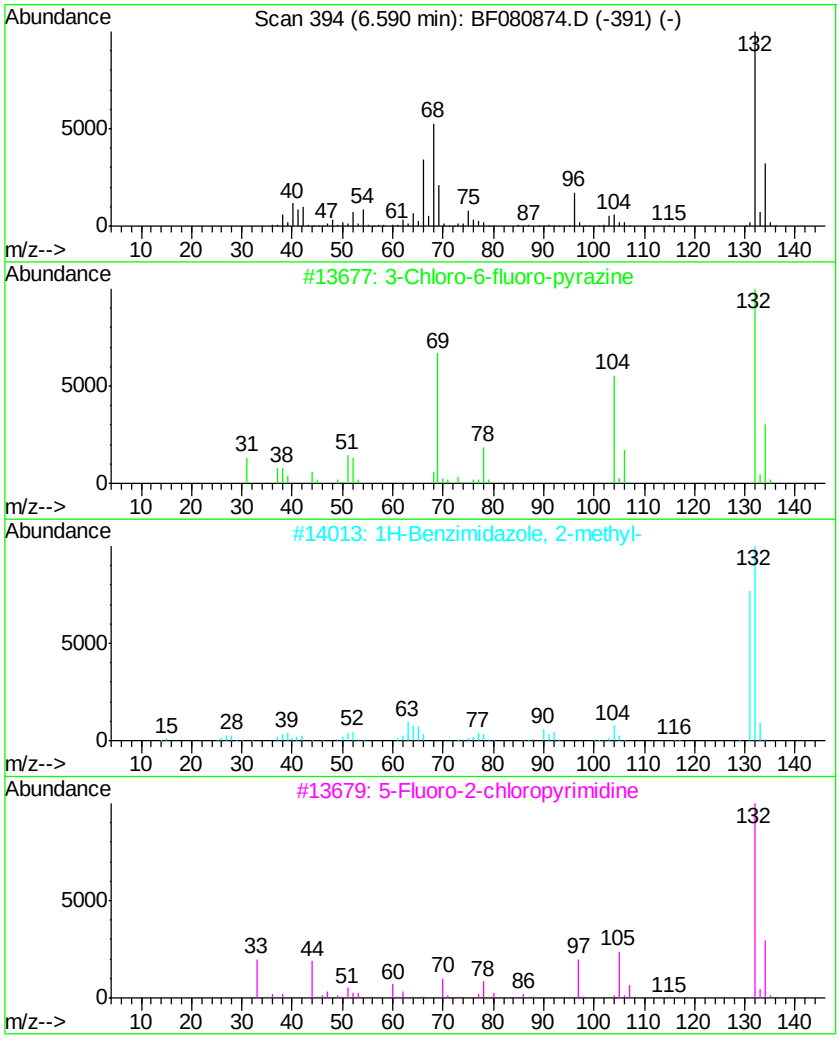
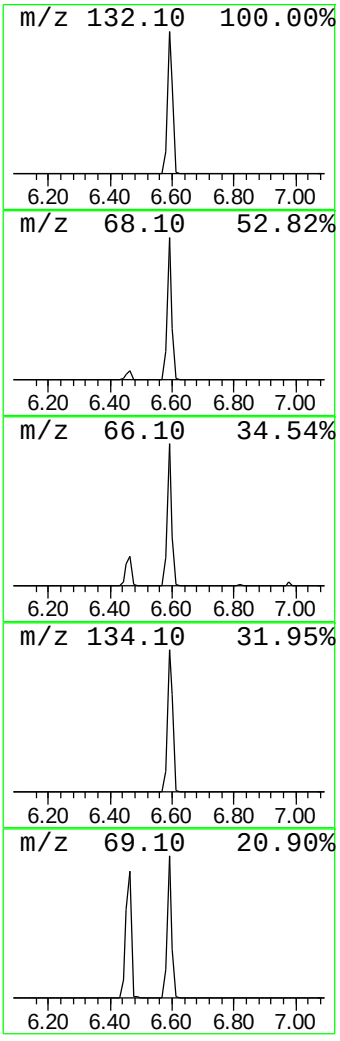
Peak Number 5 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	98.80 ng	1860810	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





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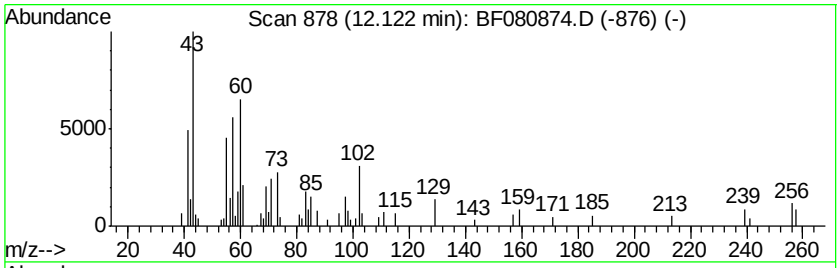
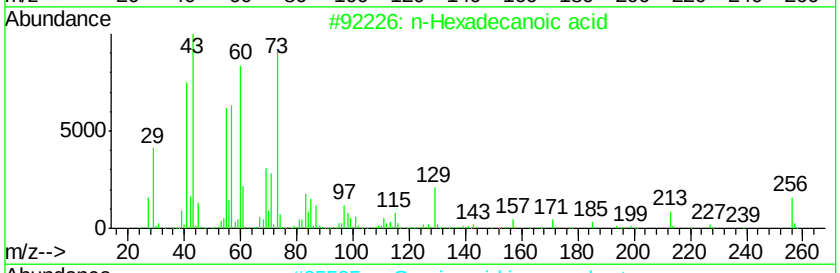
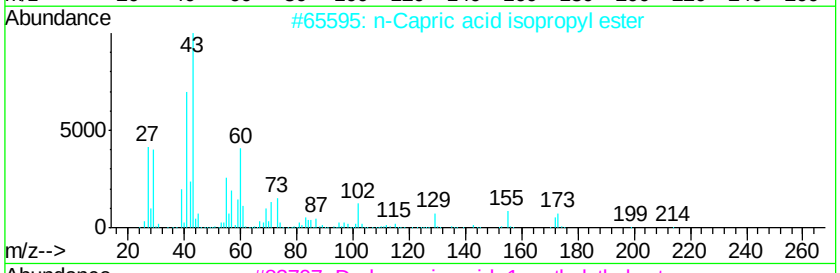
Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

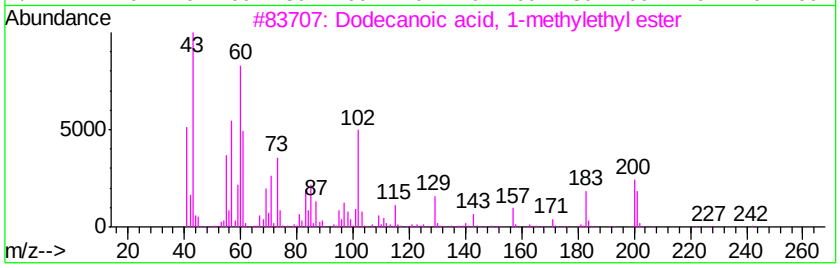
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	3.29 ng	57196	Phenanthrene-d10	11.33

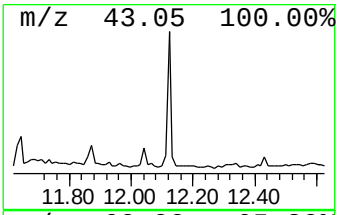
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
3	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	50
4	Isopropyl Myristate	270	C17H34O2	000110-27-0	50
5	.alpha.-D-Galactopyranoside, methyl	194	C7H14O6	003396-99-4	47

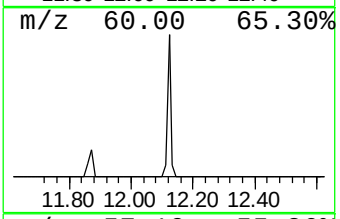


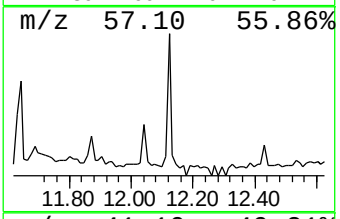


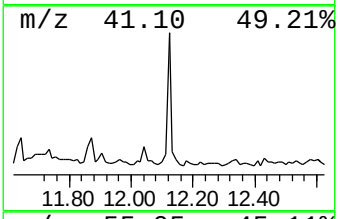


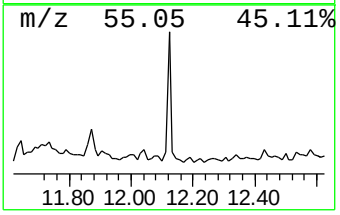












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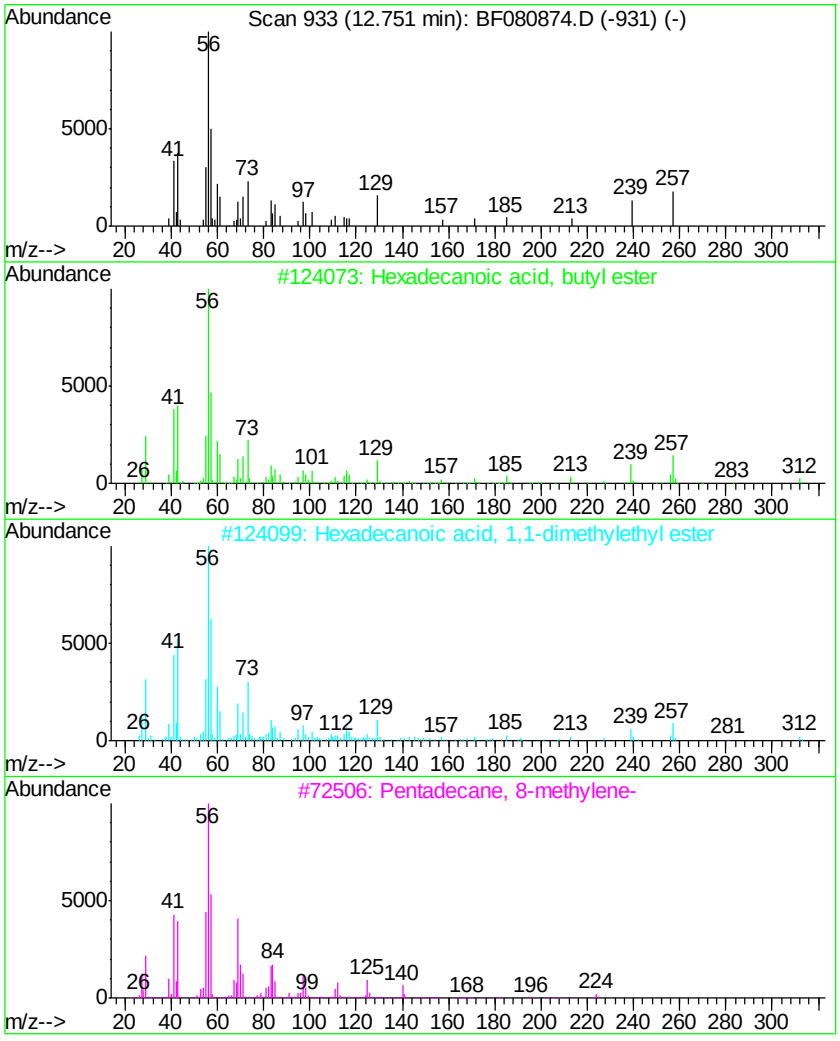
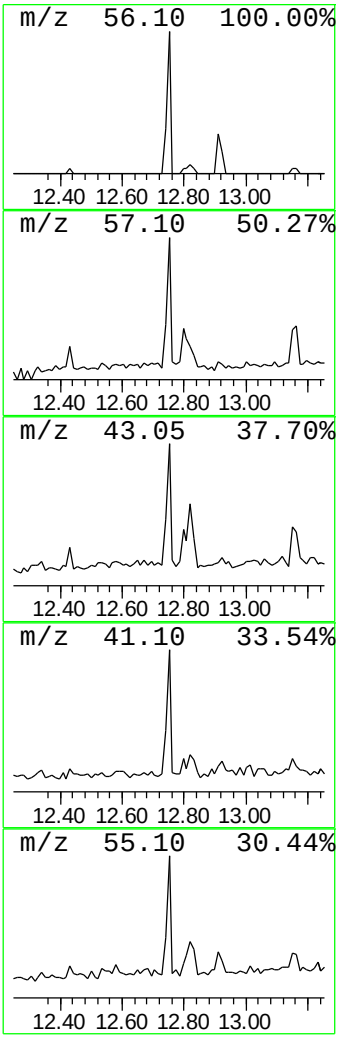
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.74 ng	46861	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	43
4	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
5	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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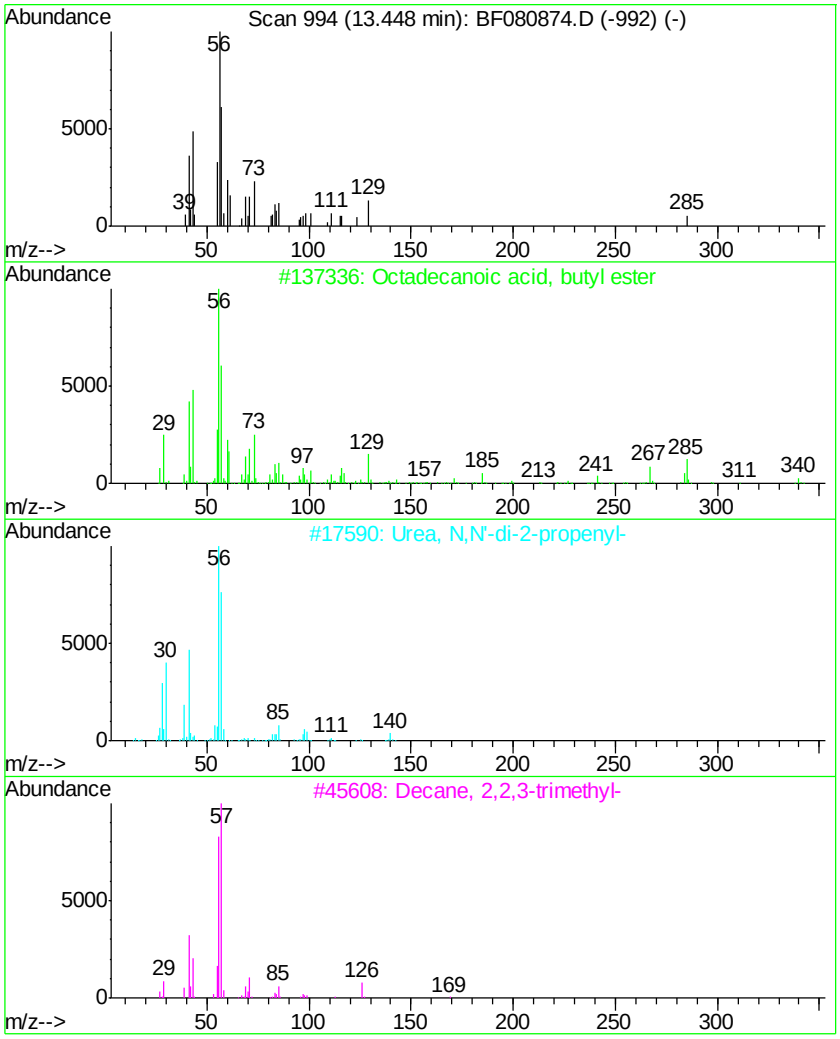
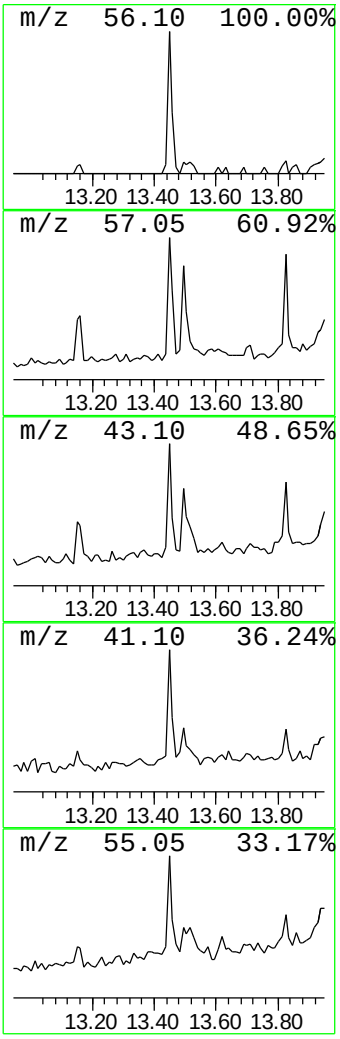
Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.29 ng	39199	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	78
2	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	43
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080874.D
Acq On : 5 Aug 2015 10:39
Operator : TP/UM
Sample : G3127-19
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EAST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.18	3.4	ng	64726	1	6.83	376680	20.0
3-Penten-2-one, 4...	4.36	4.6	ng	87211	1	6.83	376680	20.0
2-Pentanone, 4-hy...	5.02	98.4	ng	1853560	1	6.83	376680	20.0
2-Pentanone, 4-me...	5.84	3.6	ng	67489	1	6.83	376680	20.0
unknown6.59	6.59	98.8	ng	1860810	1	6.83	376680	20.0
n-Hexadecanoic acid	12.12	3.3	ng	57196	4	11.33	347512	20.0
Hexadecanoic acid...	12.75	2.7	ng	46861	5	13.96	341984	20.0
Octadecanoic acid...	13.45	2.3	ng	39199	5	13.96	341984	20.0