LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082514.D
Acq On : 24 Oct 2015 15:24
Operator : UM/IZ
Sample : G4117-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-02(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-BF101015.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	4.914	240	243	254	rBV	741069	1120631	48.68%	5.947%
2	5.360	279	282	284	rBV	1628659	1896470	82.38%	10.065%
3	5.749	314	316	319	rVB	24670	23487	1.02%	0.125%
4	6.412	371	374	376	rBV	1831769	1990371	86.46%	10.563%
5	6.526	382	384	387	rBV	2148154	1925759	83.65%	10.220%
6	6.754	402	404	407	rBV	582038	499655	21.70%	2.652%
7	6.915	415	418	420	rBV	1396193	1540877	66.93%	8.178%
8	7.326	451	454	457	rBV	1007722	1060549	46.07%	5.629%
9	8.046	514	517	519	rBV	765209	651125	28.28%	3.456%
10	9.132	609	612	614	rBV	1724837	2302099	100.00%	12.218%
11	9.520	644	646	649	rBV	329541	328204	14.26%	1.742%
12	9.806	668	671	673	rBV	586161	676897	29.40%	3.592%
13	10.229	707	708	710	rVB	35355	27970	1.21%	0.148%
14	10.595	737	740	743	rBV	1052757	975434	42.37%	5.177%
15	10.709	748	750	754	rVB	33505	49883	2.17%	0.265%
16	11.155	787	789	790	rBV	36737	33037	1.44%	0.175%
17	11.292	799	801	803	rBV	574160	565954	24.58%	3.004%
18	12.698	922	924	926	rBV	108708	89802	3.90%	0.477%
19	12.881	937	940	942	rBV	1942826	1768339	76.81%	9.385%
20	13.407	984	986	988	rBV	70429	60973	2.65%	0.324%
21	13.829	1020	1023	1031	rVB2	25809	64985	2.82%	0.345%
22	13.944	1031	1033	1036	rBV	492593	545704	23.70%	2.896%
23	14.435	1073	1076	1079	rBV2	15065	25830	1.12%	0.137%
24	14.835	1107	1111	1113	rBV	33278	48208	2.09%	0.256%
25	15.418	1159	1162	1169	rVB	388145	501740	21.79%	2.663%
26	15.853	1197	1200	1203	rBV	15223	28316	1.23%	0.150%
27	16.321	1238	1241	1249	rVB4	13849	39897	1.73%	0.212%

Sum of corrected areas: 18842196

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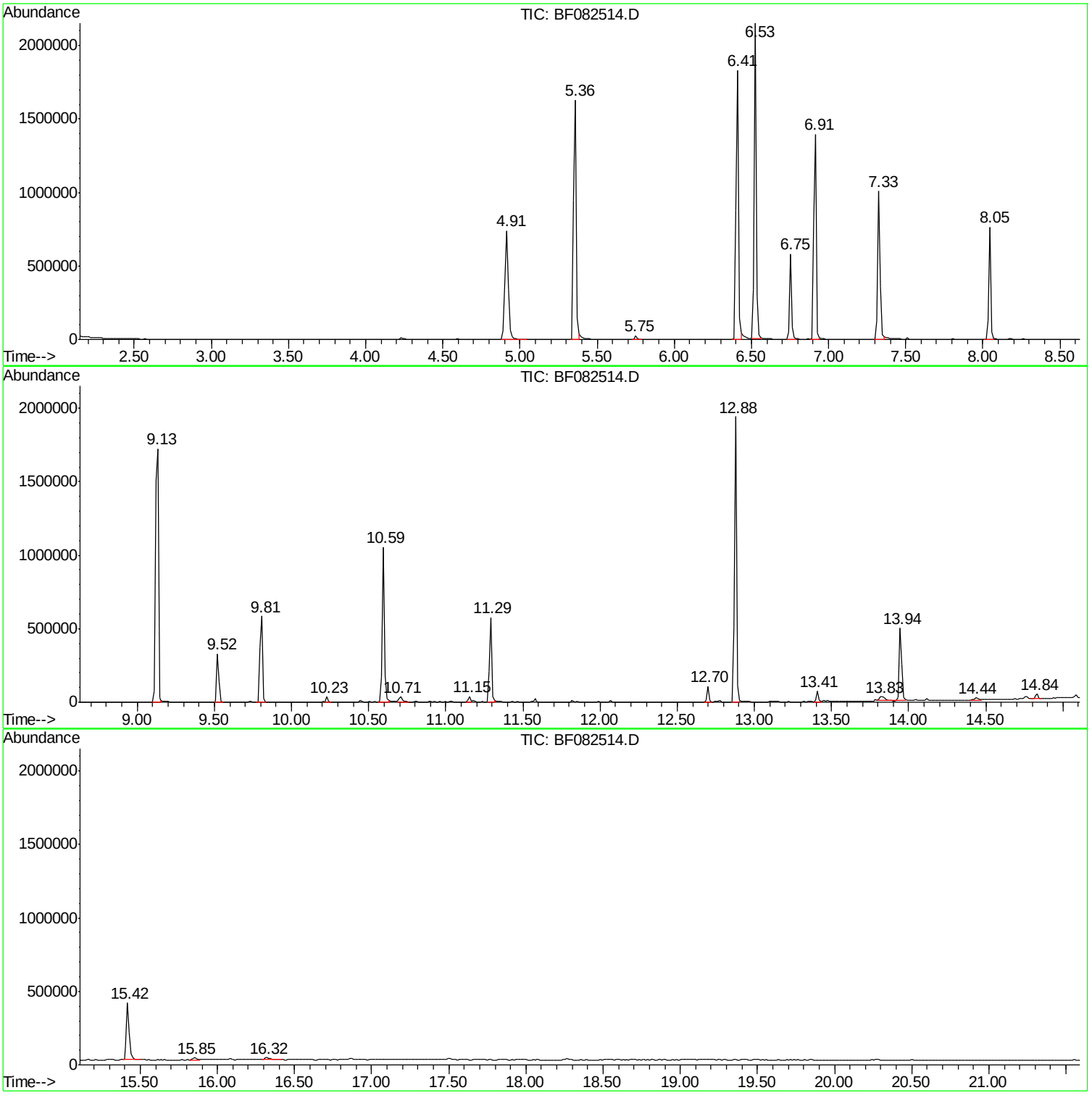
Instrument :
BNA_F
ClientSampleId :
COFF-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082514.D
Acq On : 24 Oct 2015 15:24
Operator : UM/IZ
Sample : G4117-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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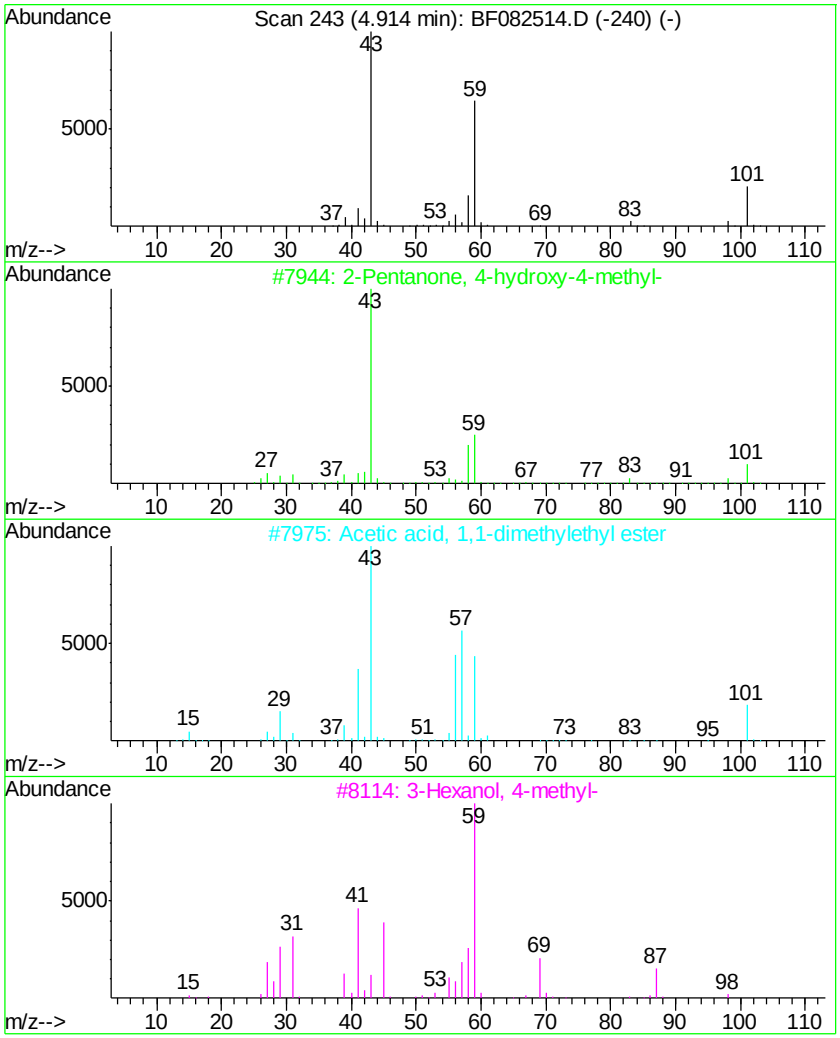
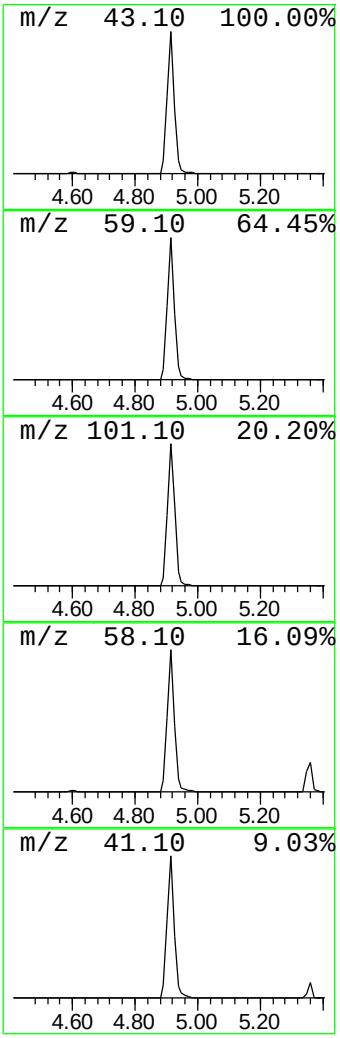
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	44.86 ng	1120630	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Acq On : 24 Oct 2015 15:24
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Sample : G4117-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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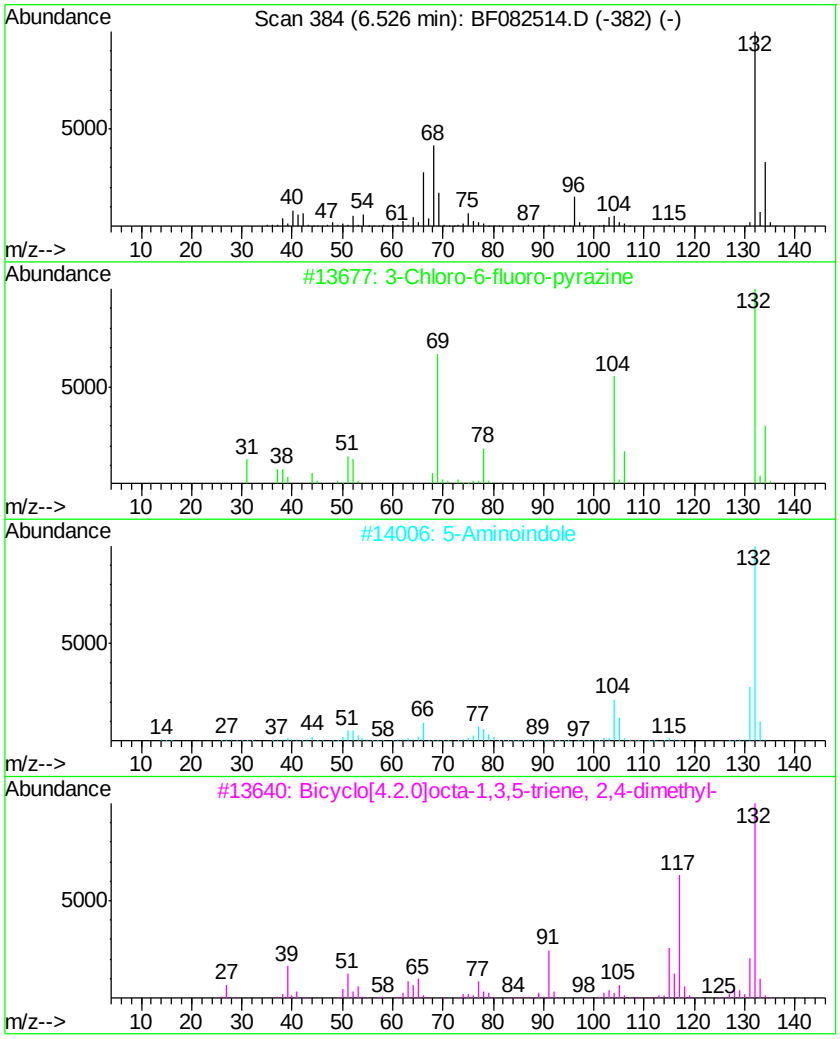
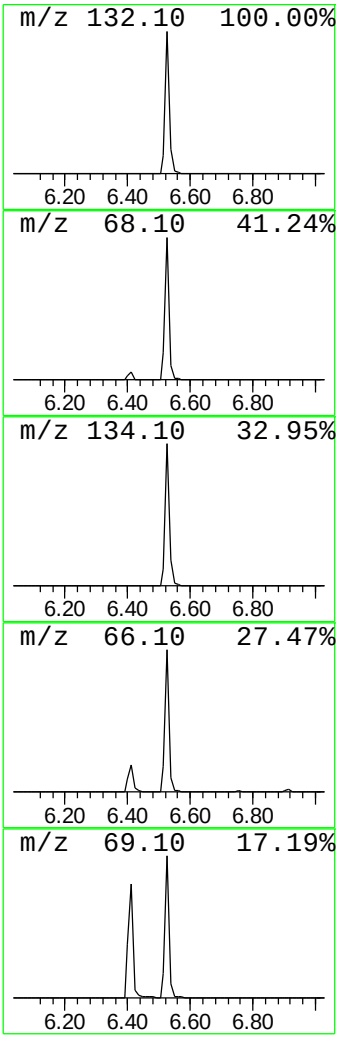
Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	77.08 ng	1925760	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : UM/IZ
Sample : G4117-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
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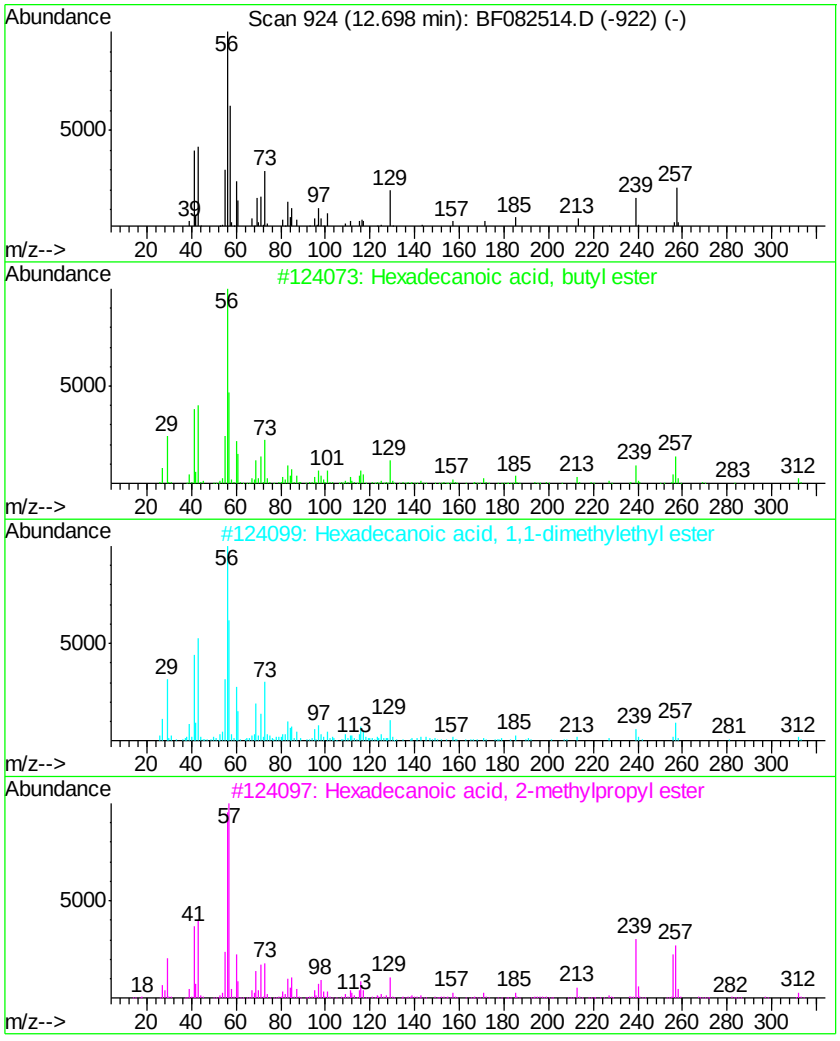
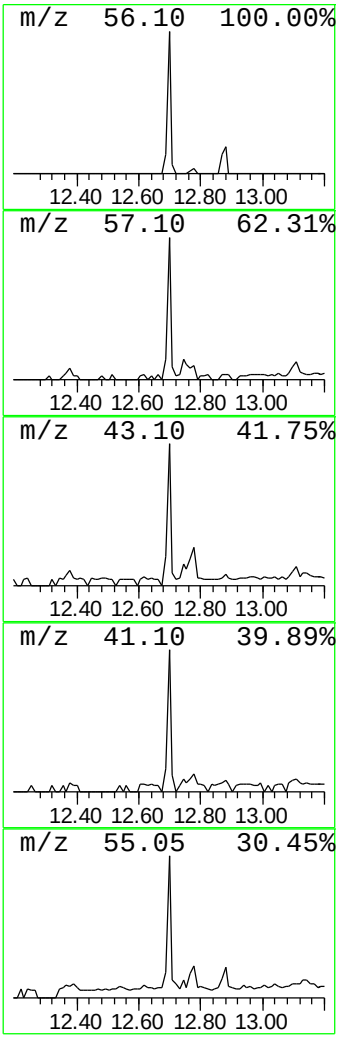
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.29 ng	89802	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	40
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	35





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Data File : BF082514.D
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Operator : UM/IZ
Sample : G4117-15
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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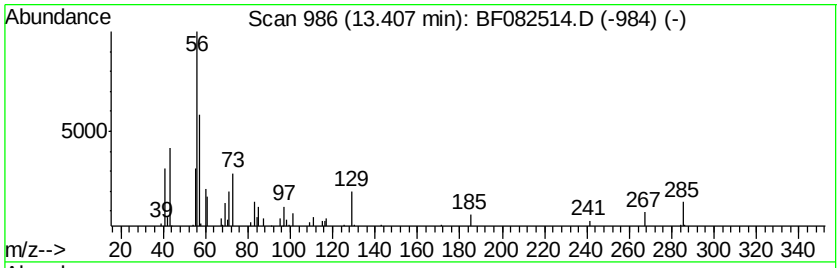
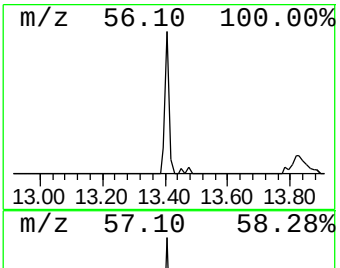
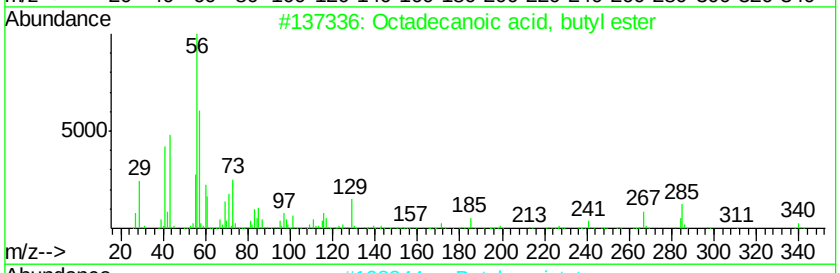
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

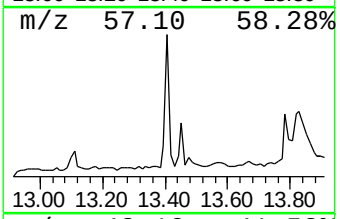
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	2.23 ng	60973	Chrysene-d12	13.94

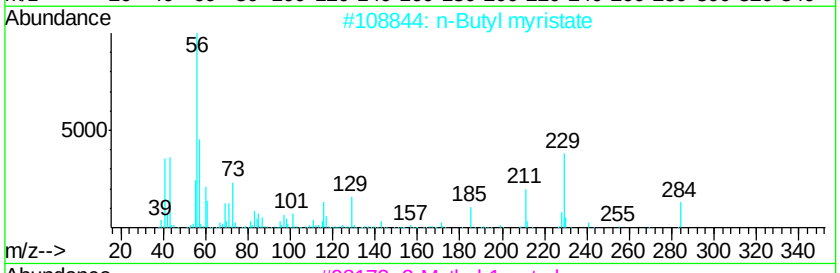
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	59
3	2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27

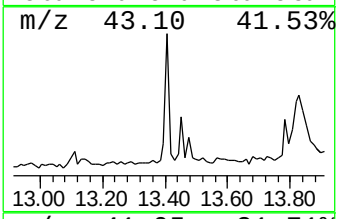


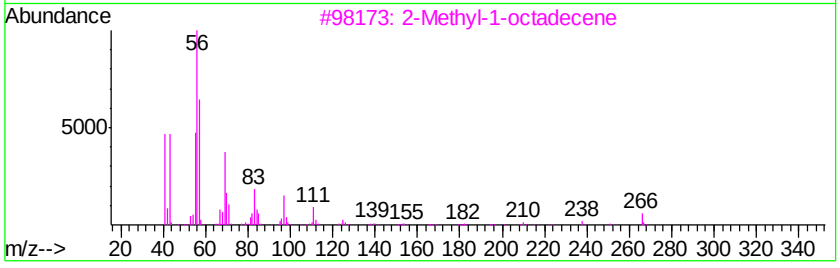


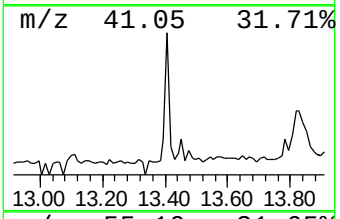


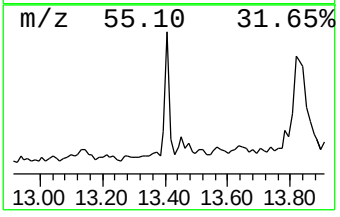












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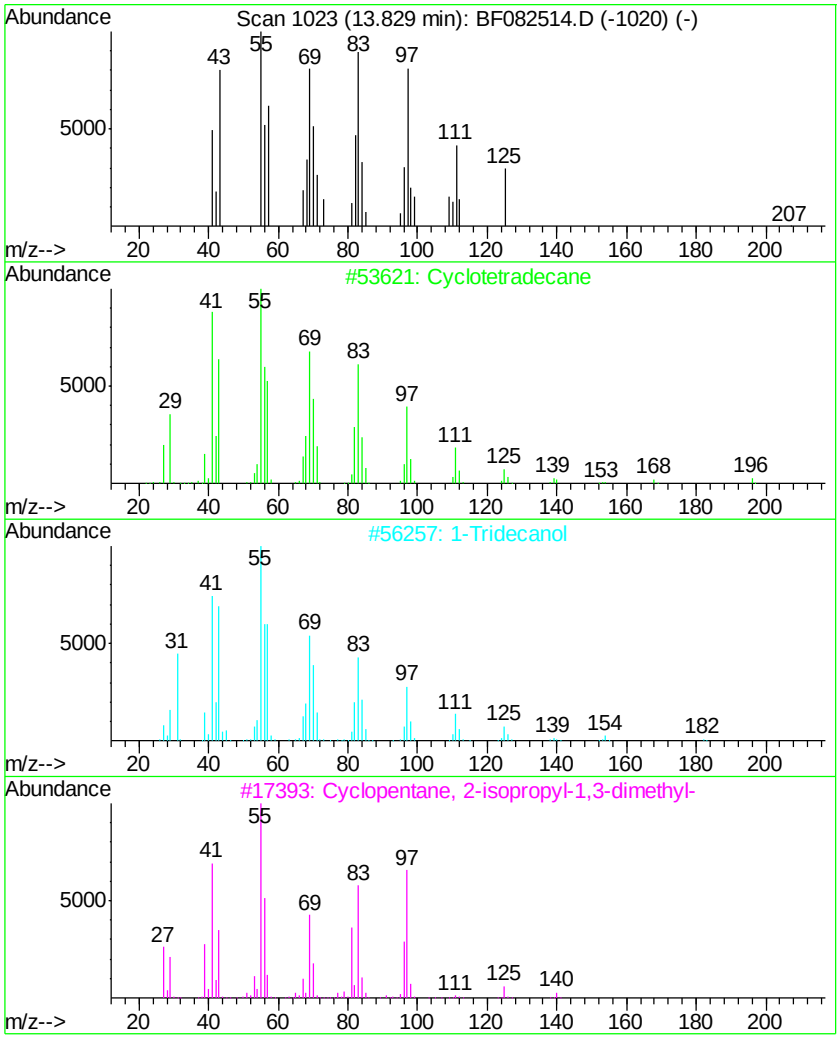
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

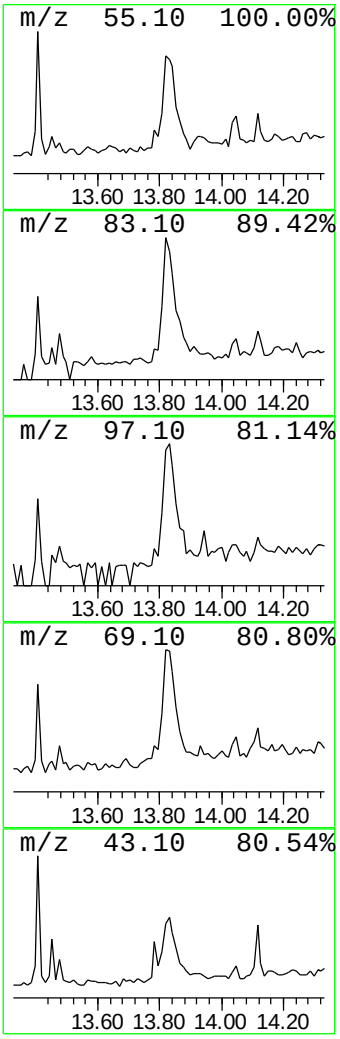
****

Peak Number 6 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.38 ng	64985	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	59
2	1-Tridecanol	200	C13H28O	000112-70-9	50
3	Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	38
4	Cycloheptane, methyl-	112	C8H16	004126-78-7	35
5	2-Cyclohexen-1-ol, 1-methyl-	112	C7H12O	023758-27-2	35





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.91	44.9	ng	1120630	1	6.75	499655	20.0
unknown6.53	6.53	77.1	ng	1925760	1	6.75	499655	20.0
Hexadecanoic acid...	12.70	3.3	ng	89802	5	13.94	545704	20.0
Octadecanoic acid...	13.41	2.2	ng	60973	5	13.94	545704	20.0
Cyclotetradecane	13.83	2.4	ng	64985	5	13.94	545704	20.0