LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082509.D
Acq On : 24 Oct 2015 13:00
Operator : UM/IZ
Sample : G4119-13
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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	3.177	87	91	97	rVB	25553	50052	2.36%	0.281%
2	4.229	180	183	194	rBV	676601	933024	43.96%	5.233%
3	4.937	240	245	247	rBV	1070542	2122212	100.00%	11.903%
4	5.360	279	282	285	rBV	683649	731150	34.45%	4.101%
5	5.417	285	287	293	rVB	37008	48587	2.29%	0.273%
6	5.749	314	316	318	rVB	24440	21720	1.02%	0.122%
7	6.412	372	374	382	rBV	1328180	1427650	67.27%	8.007%
8	6.526	382	384	387	rBV	1231646	1097665	51.72%	6.157%
9	6.755	402	404	407	rBV	708176	592520	27.92%	3.323%
10	6.915	415	418	420	rBV	1241787	1345224	63.39%	7.545%
11	7.326	452	454	457	rBV	907338	881240	41.52%	4.943%
12	8.046	514	517	519	rBV	898738	775226	36.53%	4.348%
13	9.132	609	612	614	rBV	1271791	1791925	84.44%	10.051%
14	9.521	644	646	649	rBV	346190	415827	19.59%	2.332%
15	9.738	663	665	667	rVB	20459	26860	1.27%	0.151%
16	9.806	668	671	673	rBV	821065	793833	37.41%	4.452%
17	10.206	704	706	707	rBV	21267	21354	1.01%	0.120%
18	10.229	707	708	712	rVV	65968	58687	2.77%	0.329%
19	10.355	715	719	721	rBV2	12551	22792	1.07%	0.128%
20	10.446	725	727	731	rBV	25866	41501	1.96%	0.233%
21	10.595	736	740	743	rBV	261062	252421	11.89%	1.416%
22	10.709	748	750	753	rBV	89878	127231	6.00%	0.714%
23	11.155	787	789	790	rBV	81796	72483	3.42%	0.407%
24	11.178	790	791	794	rVB2	33865	41950	1.98%	0.235%
25	11.292	799	801	802	rBV	738139	666407	31.40%	3.738%
26	11.315	802	803	805	rVV	107421	92558	4.36%	0.519%
27	11.372	805	808	809	rVB2	12800	22247	1.05%	0.125%
28	11.532	820	822	825	rBV2	27216	46521	2.19%	0.261%
29	11.578	825	826	829	rVB	66119	60693	2.86%	0.340%
30	11.818	846	847	851	rVV	31330	47497	2.24%	0.266%
31	11.898	853	854	858	rVB3	18700	35482	1.67%	0.199%
32	11.989	860	862	864	rBV	49583	41430	1.95%	0.232%
33	12.378	894	896	898	rBV	41455	37270	1.76%	0.209%
34	12.504	906	907	909	rBV	70222	62677	2.95%	0.352%

LSC Area Percent Report

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Data File : BF082509.D
Acq On : 24 Oct 2015 13:00
Operator : UM/IZ
Sample : G4119-13
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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

35	12.732	925	927	930	rBV2	67816	107701	5.07%	0.604%
36	12.778	930	931	934	rVB3	15304	23291	1.10%	0.131%
37	12.881	937	940	943	rBV	1434702	1322644	62.32%	7.418%
38	13.109	958	960	962	rBV	35308	46805	2.21%	0.263%
39	13.464	989	991	993	rBV	32868	35760	1.69%	0.201%
40	13.830	1019	1023	1027	rVB3	42791	114314	5.39%	0.641%
41	13.967	1033	1035	1038	rBV	448810	678852	31.99%	3.808%
42	14.150	1049	1051	1057	rVB2	28976	42076	1.98%	0.236%
43	15.487	1165	1168	1175	rVB	433154	610660	28.77%	3.425%
44	15.921	1204	1206	1208	rBV	27660	41092	1.94%	0.230%

Sum of corrected areas: 17829111

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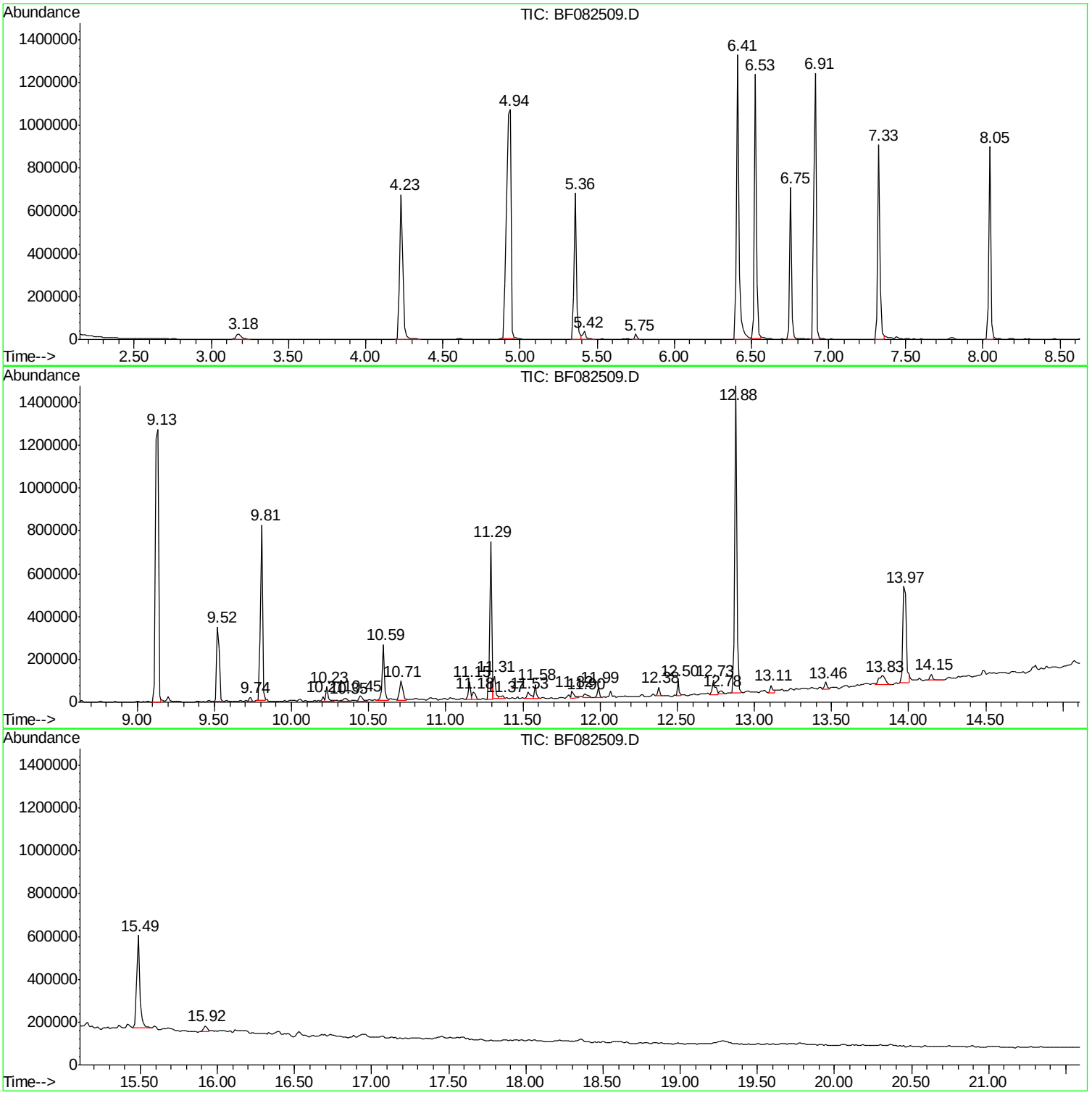
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB15-08-10-10.5

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082509.D
Acq On : 24 Oct 2015 13:00
Operator : UM/IZ
Sample : G4119-13
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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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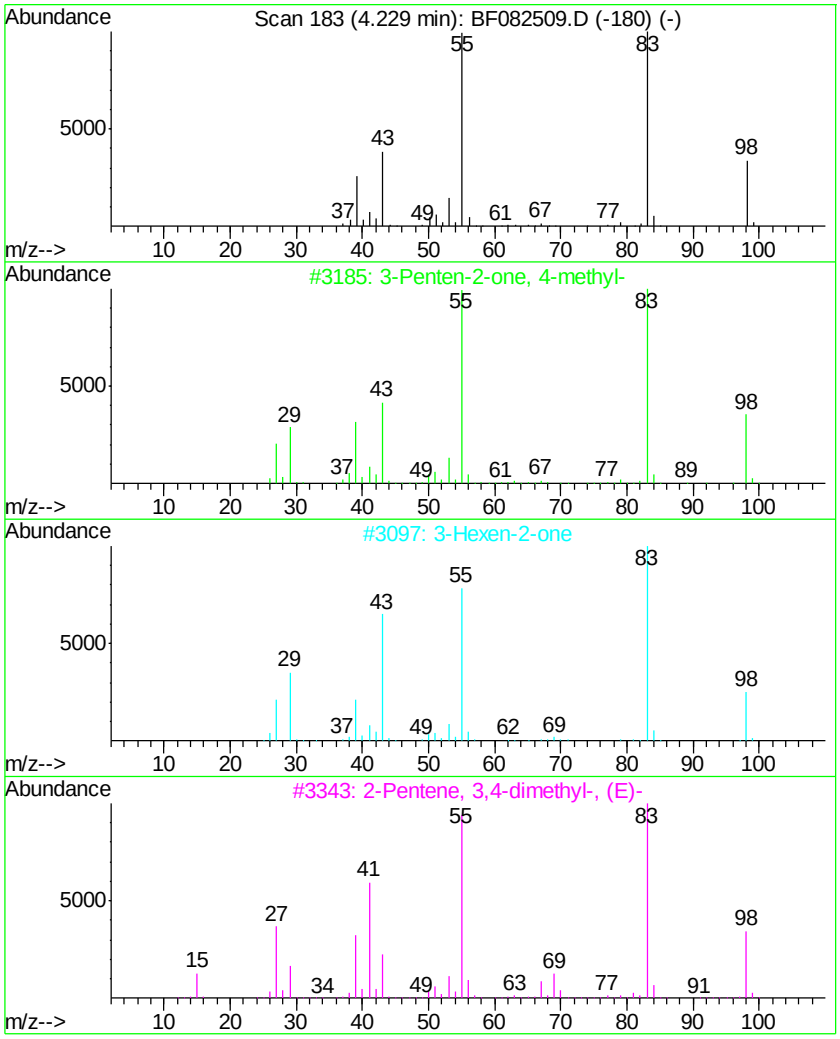
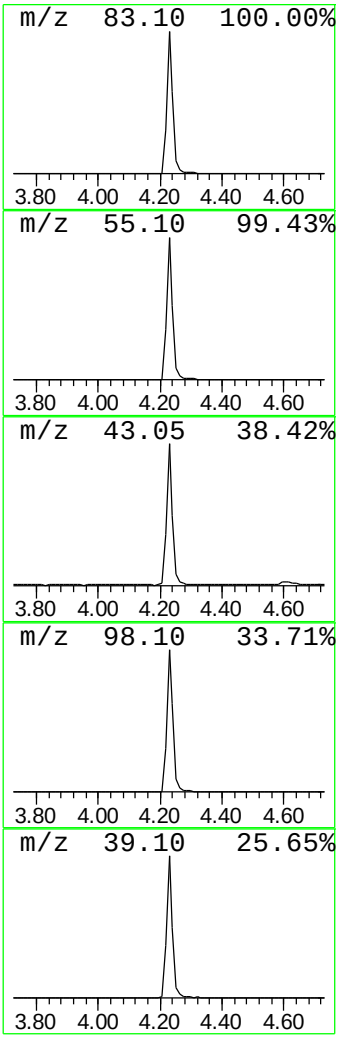
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.23	31.49 ng	933024	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082509.D
Acq On : 24 Oct 2015 13:00
Operator : UM/IZ
Sample : G4119-13
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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

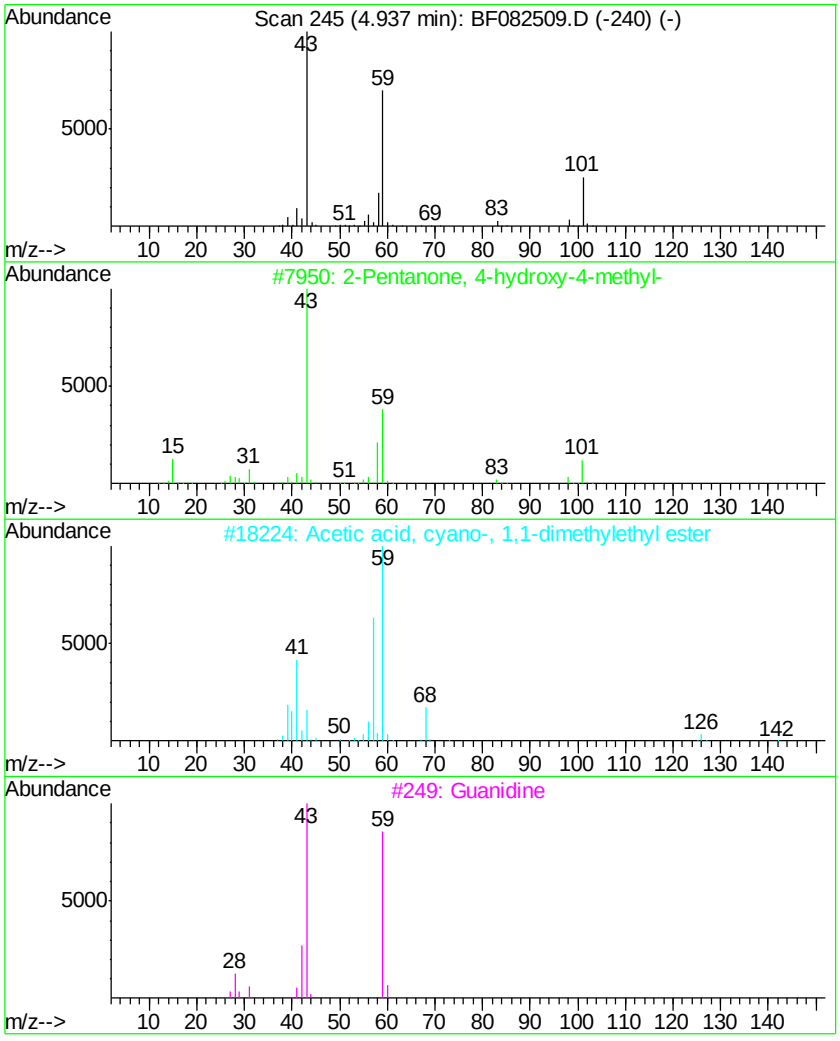
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

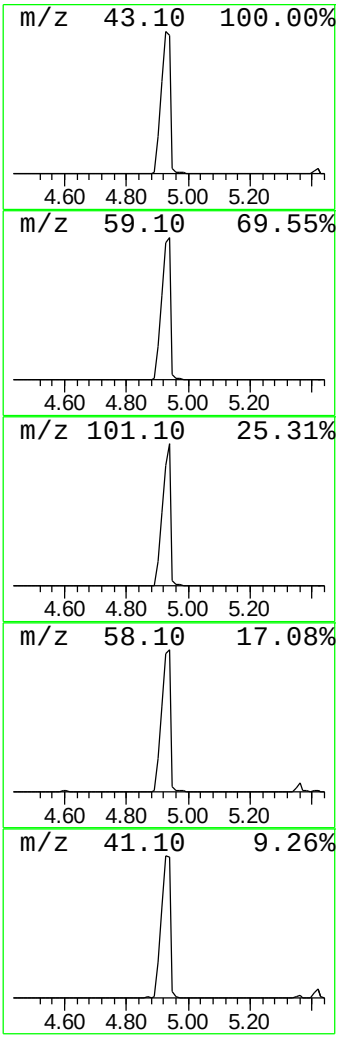
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	71.63 ng	2122210	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	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Guanidine	59	CH5N3	000113-00-8	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BF082509.D
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Operator : UM/IZ
Sample : G4119-13
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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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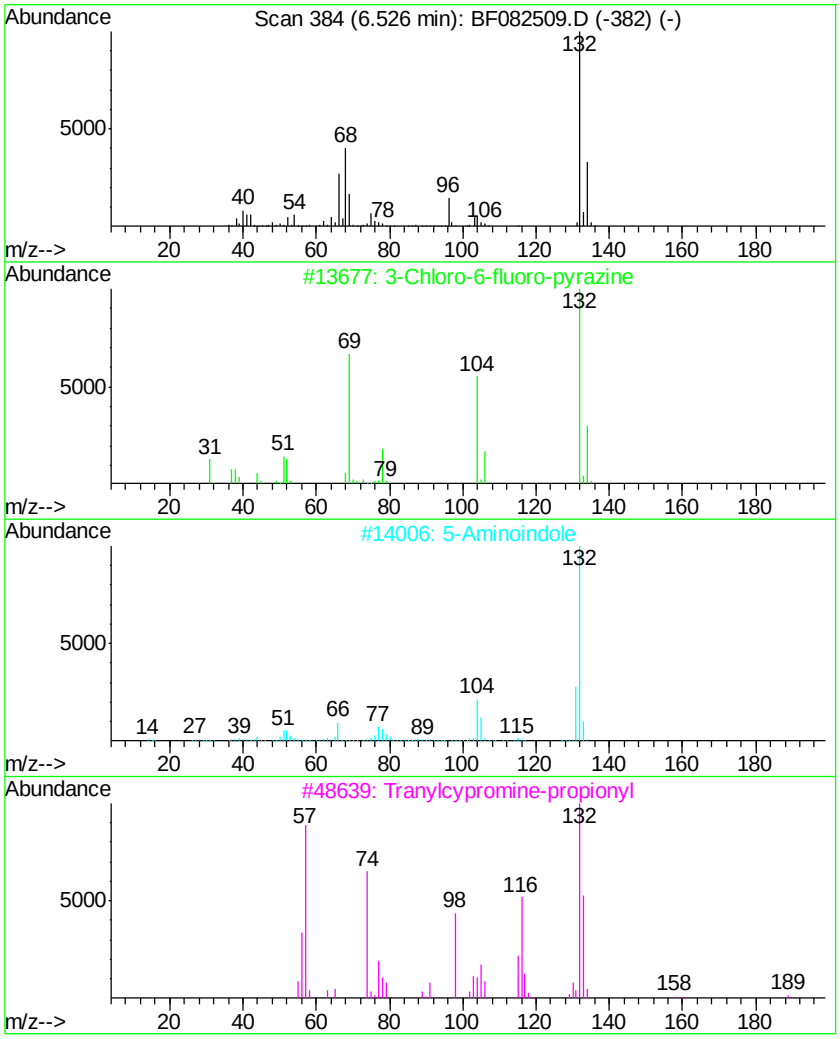
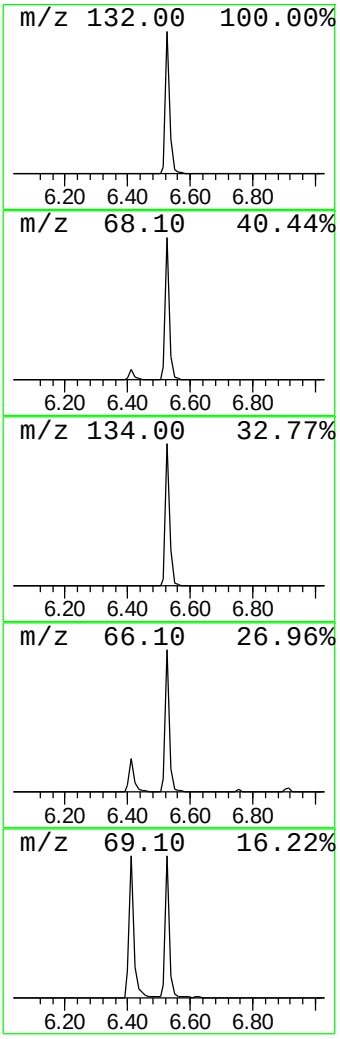
Peak Number 3 unknown6.53 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	37.05 ng	1097670	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : G4119-13
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Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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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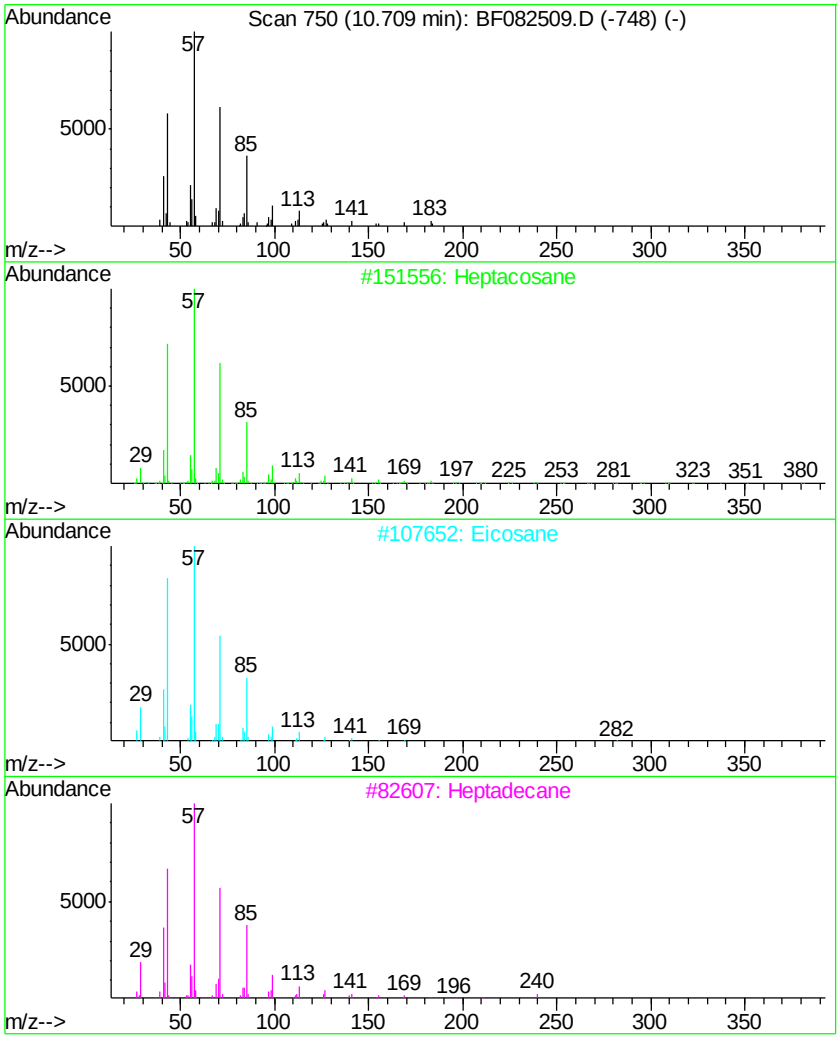
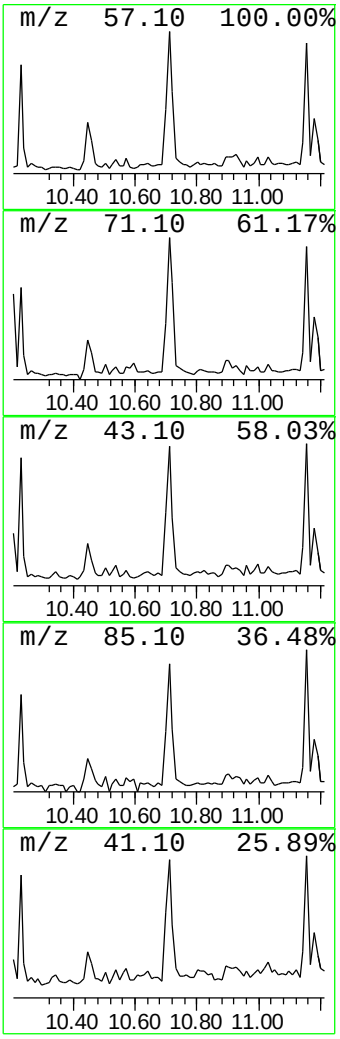
Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	3.82 ng	127231	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Tridecane	184	C13H28	000629-50-5	87
5	Tetracosane	338	C24H50	000646-31-1	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082509.D
Acq On : 24 Oct 2015 13:00
Operator : UM/IZ
Sample : G4119-13
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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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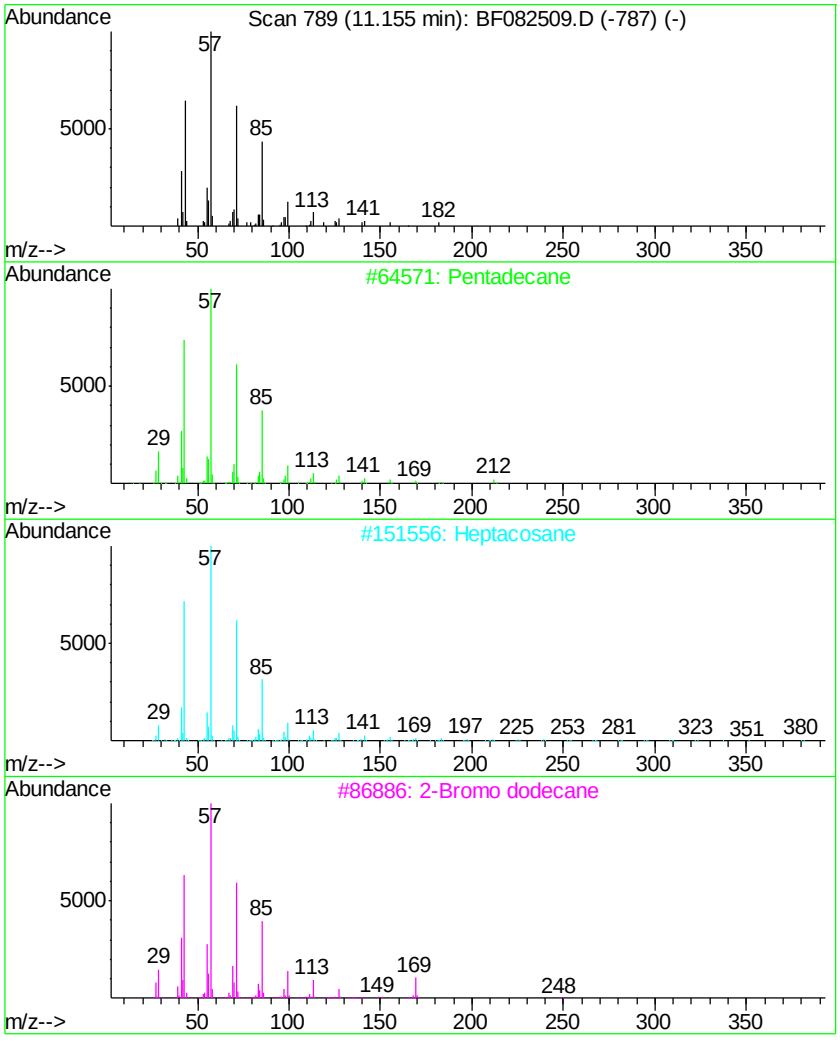
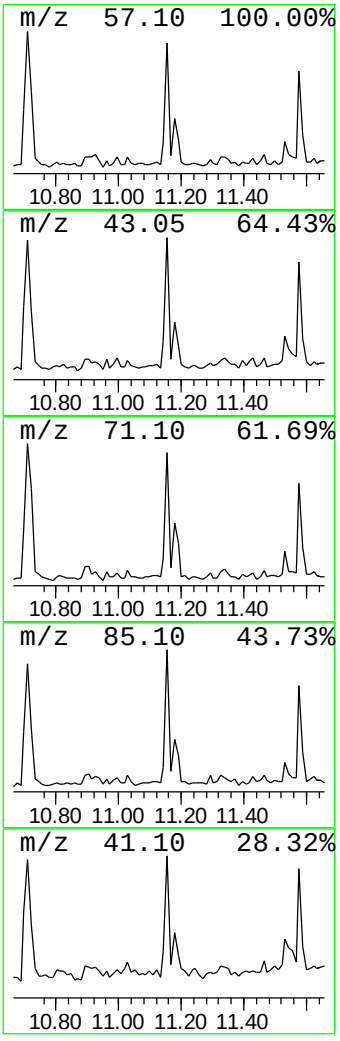
Peak Number 6 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	2.18 ng	72483	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetradecane	198	C14H30	000629-59-4	87





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Acq On : 24 Oct 2015 13:00
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Misc :
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Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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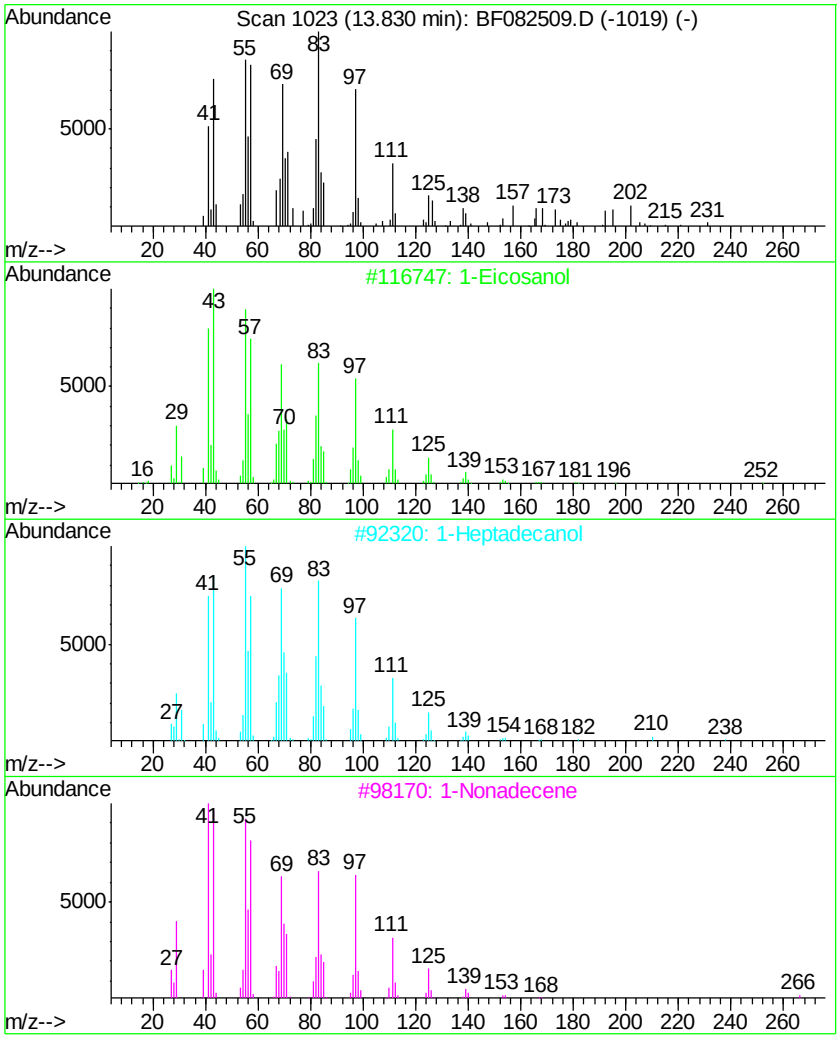
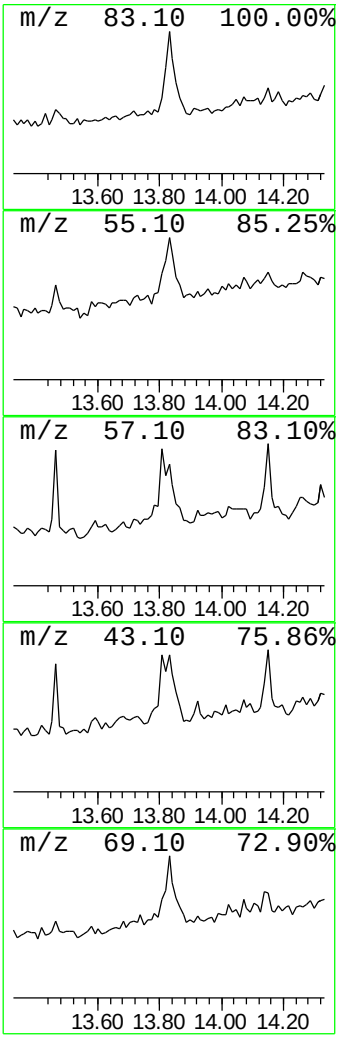
Peak Number 7 1-Eicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.37 ng	114314	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	91
2	1-Heptadecanol	256	C17H36O	001454-85-9	90
3	1-Nonadecene	266	C19H38	018435-45-5	68
4	1-Octadecanol	270	C18H38O	000112-92-5	64
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	62





Tentatively Identified Compound (LSC) summary

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Acq On : 24 Oct 2015 13:00
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Sample : G4119-13
Misc :
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Instrument : BNA_F
ClientSampleId : SB15-08-10-10.5

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.23	31.5	ng	933024	1	6.75	592520	20.0
2-Pentanone, 4-hy...	4.94	71.6	ng	2122210	1	6.75	592520	20.0
unknown6.53	6.53	37.0	ng	1097670	1	6.75	592520	20.0
Heptacosane	10.71	3.8	ng	127231	4	11.29	666407	20.0
Pentadecane	11.16	2.2	ng	72483	4	11.29	666407	20.0
1-Eicosanol	13.83	3.4	ng	114314	5	13.98	678852	20.0