LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

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-BF110715.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	4.967	249	252	255	rVB	854033	913503	14.21%	2.052%
2	5.413	289	291	294	rBV	1923536	2210409	34.37%	4.965%
3	6.453	380	382	384	rBV	1749587	1415550	22.01%	3.180%
4	6.579	390	393	395	rBV	5004666	4595500	71.47%	10.323%
5	6.796	410	412	414	rBV	938019	1183752	18.41%	2.659%
6	6.876	417	419	424	rBV	68224	81459	1.27%	0.183%
7	6.956	424	426	429	rBV	3388265	4436230	68.99%	9.965%
8	7.367	459	462	465	rBV	3378566	3596608	55.93%	8.079%
9	7.482	467	472	475	rBV	76233	116200	1.81%	0.261%
10	7.836	500	503	505	rBV	143050	183632	2.86%	0.412%
11	8.008	516	518	519	rBV	52013	70002	1.09%	0.157%
12	8.088	523	525	529	rBV	1761651	1642240	25.54%	3.689%
13	8.590	568	569	572	rBV	49943	73615	1.14%	0.165%
14	8.808	585	588	589	rVB	58821	72620	1.13%	0.163%
15	8.899	594	596	599	rBV2	104859	138330	2.15%	0.311%
16	9.048	607	609	612	rVB	150244	140509	2.19%	0.316%
17	9.173	617	620	622	rBV	6998920	6430284	100.00%	14.444%
18	9.425	640	642	645	rBV2	74366	115094	1.79%	0.259%
19	9.505	645	649	650	rBV	166453	182439	2.84%	0.410%
20	9.562	653	654	657	rVB	421826	336631	5.24%	0.756%
21	9.619	657	659	662	rBV2	61108	100287	1.56%	0.225%
22	9.848	676	679	681	rBV	1778446	1739541	27.05%	3.907%
23	10.053	694	697	699	rBV2	42909	82904	1.29%	0.186%
24	10.259	713	715	719	rVB3	124210	190447	2.96%	0.428%
25	10.339	719	722	723	rBV	102351	99849	1.55%	0.224%
26	10.454	730	732	735	rBV	58652	71757	1.12%	0.161%
27	10.636	745	748	750	rBV	3611410	3467739	53.93%	7.790%
28	10.762	757	759	763	rVB	76796	103625	1.61%	0.233%
29	10.854	765	767	770	rBV2	56232	69114	1.07%	0.155%
30	11.105	787	789	792	rVB	205801	184643	2.87%	0.415%
31	11.208	796	798	800	rBV	116995	100186	1.56%	0.225%
32	11.322	806	808	811	rVB2	1341697	1475653	22.95%	3.315%
33	11.562	826	829	833	rVB2	62655	107304	1.67%	0.241%
34	11.631	833	835	838	rBV	64287	68598	1.07%	0.154%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

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-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.722	842	843	846	rVB	146911	123923	1.93%	0.278%
36	11.825	847	852	854	rBV2	69254	79066	1.23%	0.178%
37	11.894	857	858	860	rVB	250376	256596	3.99%	0.576%
38	12.168	880	882	884	rVB	135524	110596	1.72%	0.248%
39	12.922	945	948	950	rBV	4534365	5258860	81.78%	11.813%
40	13.825	1024	1027	1030	rBV2	70582	89830	1.40%	0.202%
41	13.962	1037	1039	1041	rBV	1262891	1124339	17.49%	2.526%
42	14.831	1112	1115	1116	rBV	78880	110919	1.72%	0.249%
43	15.391	1161	1164	1166	rBV	812228	1098473	17.08%	2.467%
44	15.437	1166	1168	1171	rVB	52697	70847	1.10%	0.159%
45	15.848	1202	1204	1207	rVB	52964	74780	1.16%	0.168%
46	16.317	1243	1245	1251	rVB	58650	112512	1.75%	0.253%
47	16.877	1291	1294	1297	rBV	47772	89800	1.40%	0.202%
48	17.529	1348	1351	1357	rVB3	46863	121307	1.89%	0.272%

Sum of corrected areas: 44518102

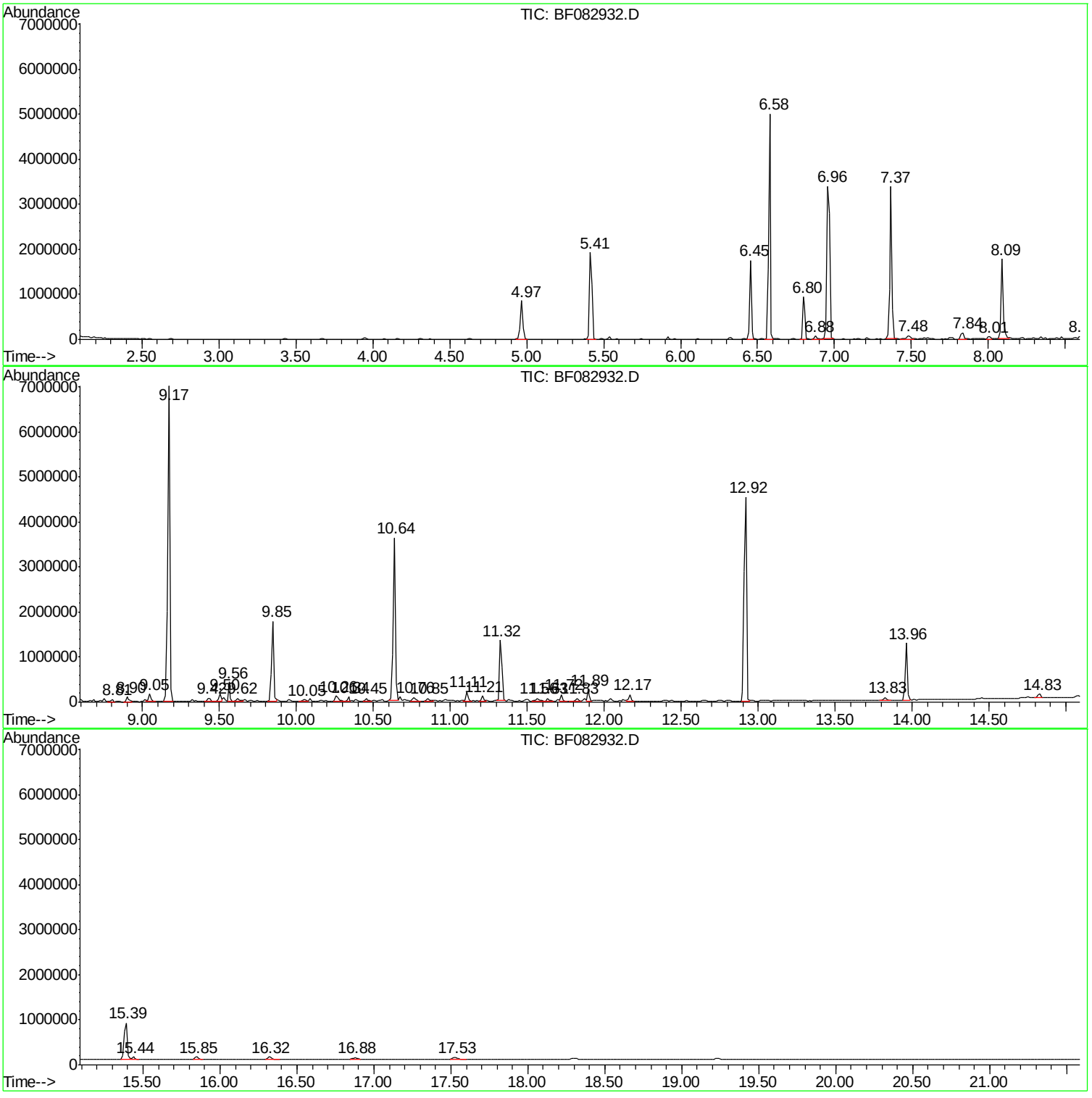
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

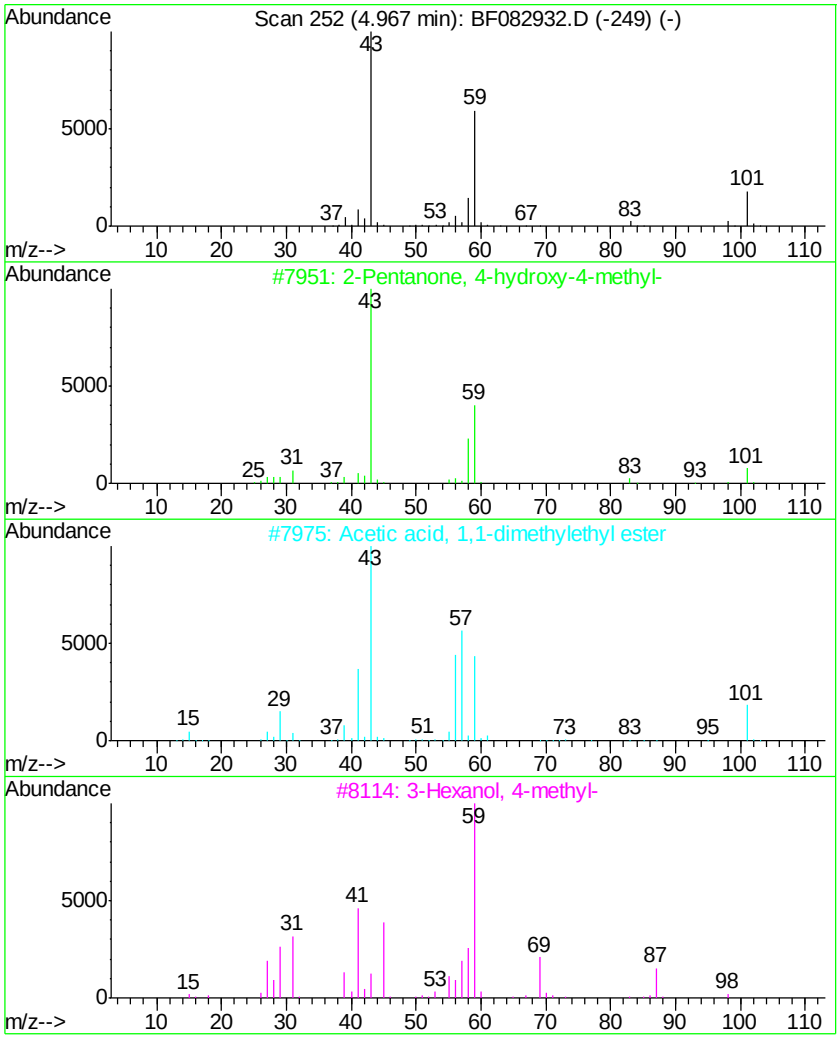
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

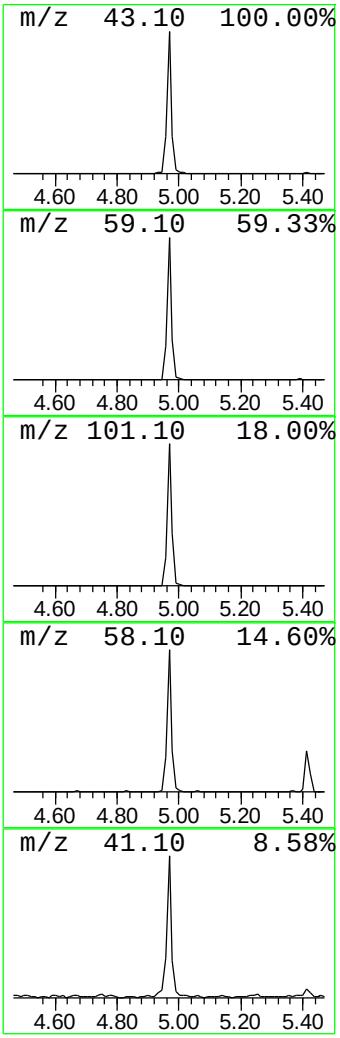
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	15.43 ng	913503	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

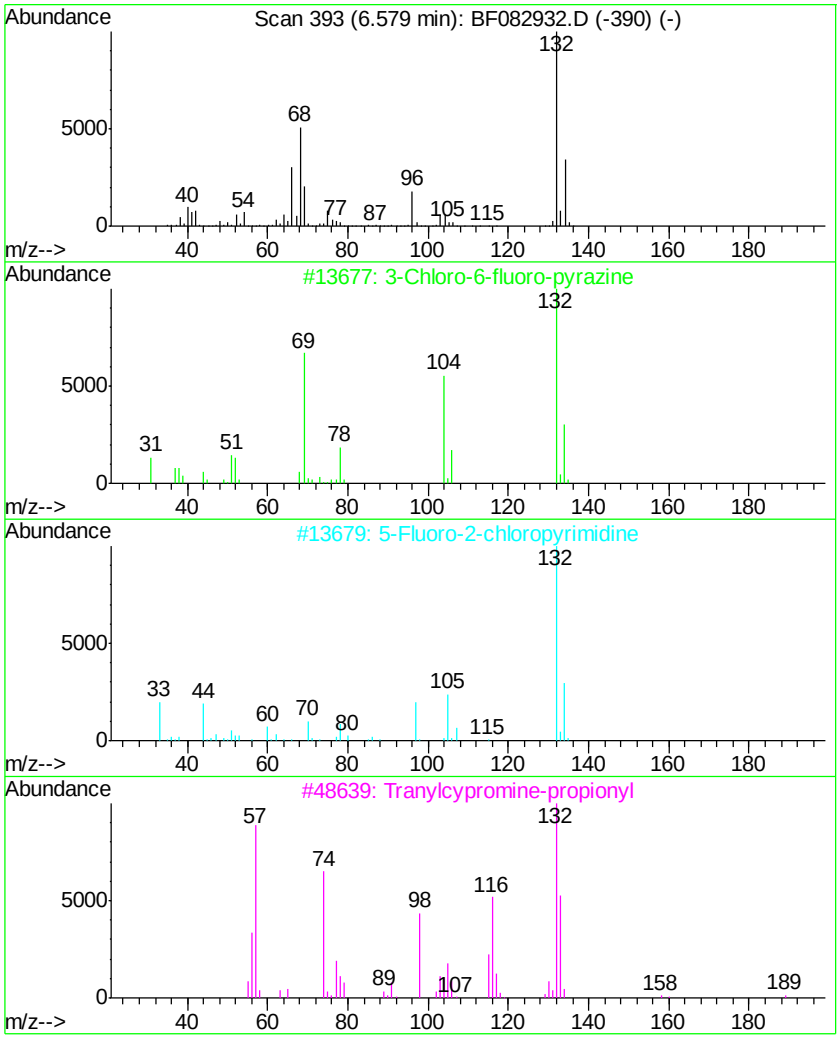
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

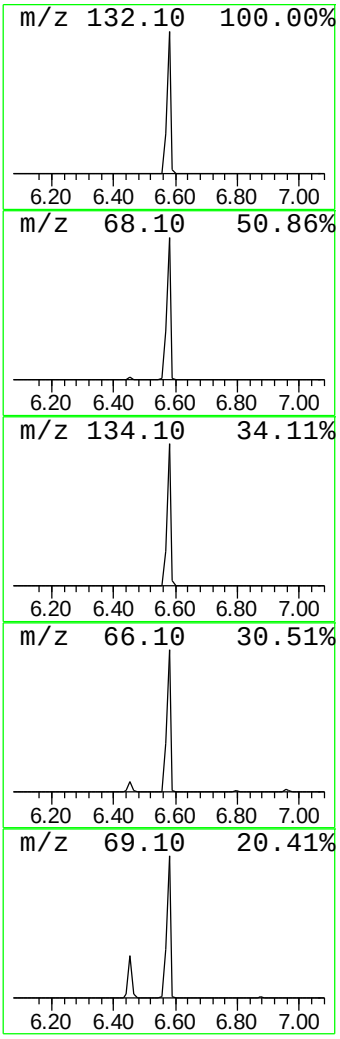
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	77.64 ng	4595500	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

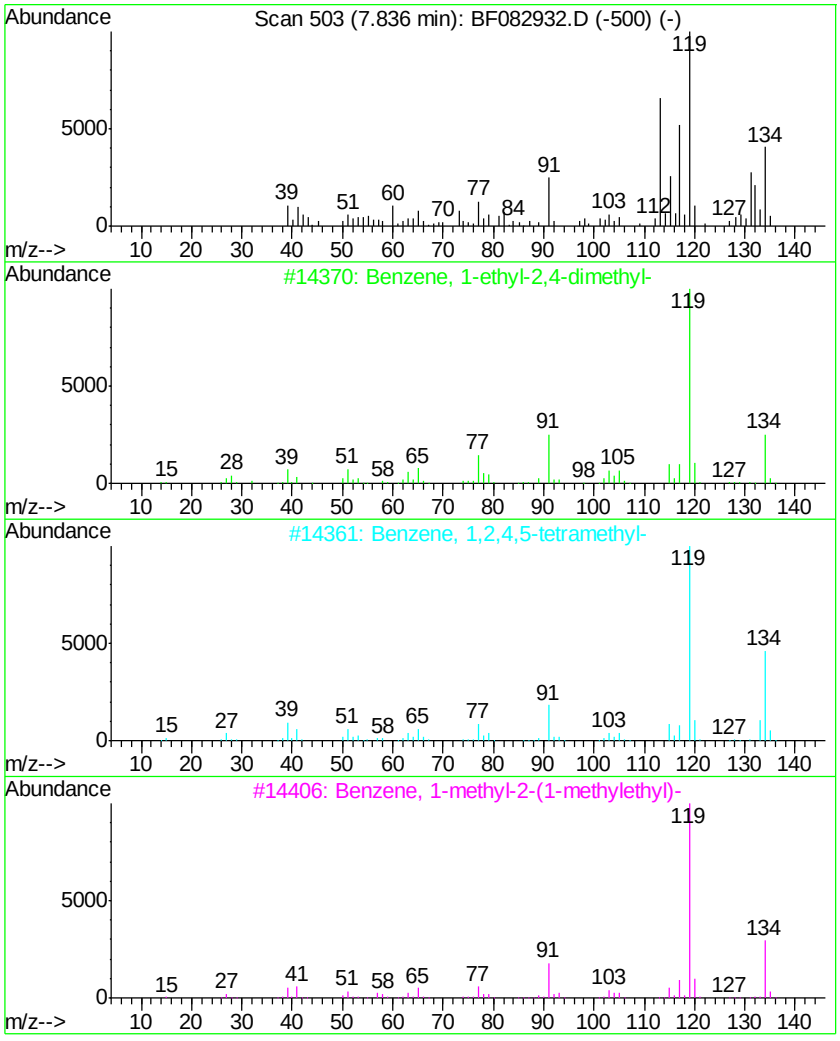
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

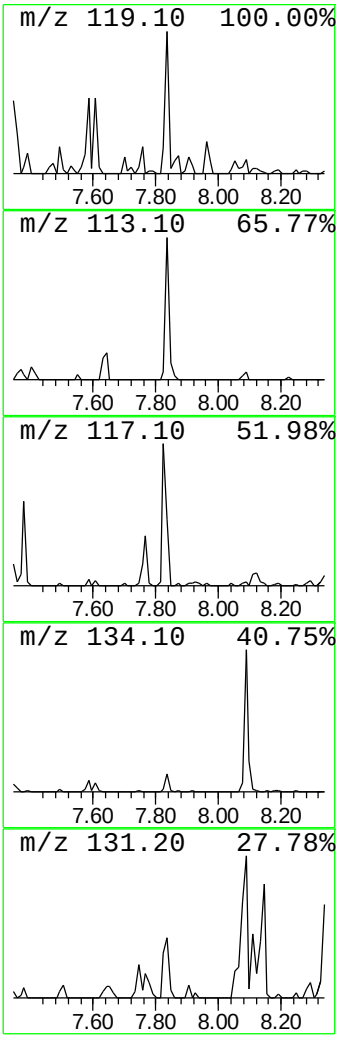
****

Peak Number 4 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	2.24 ng	183632	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	50
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	50
3	Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	50
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	46
5	Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

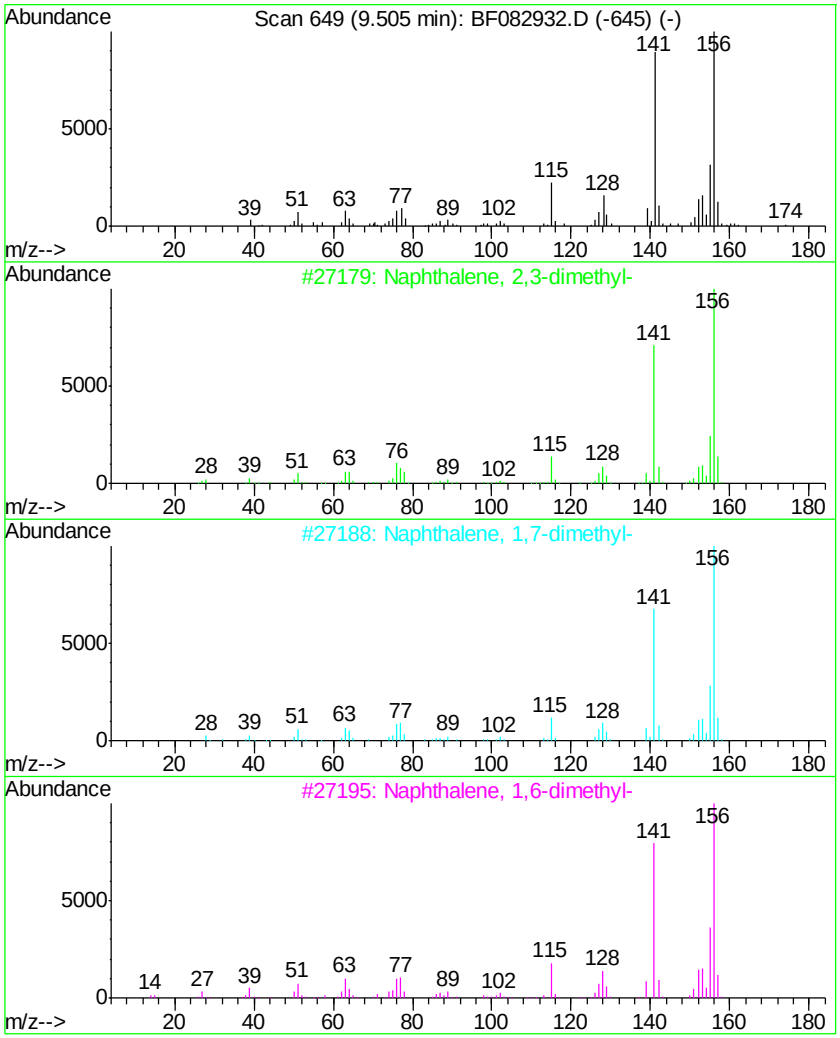
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

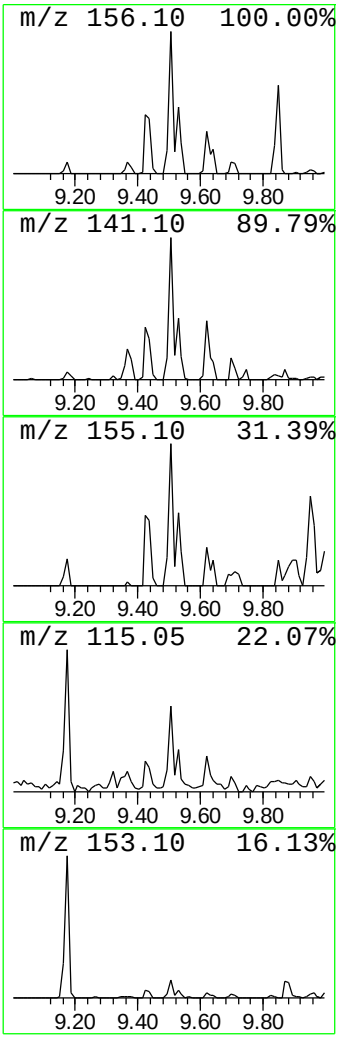
****

Peak Number 5 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	2.10 ng	182439	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

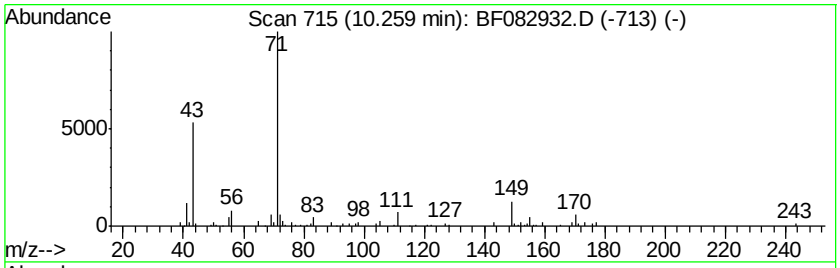
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

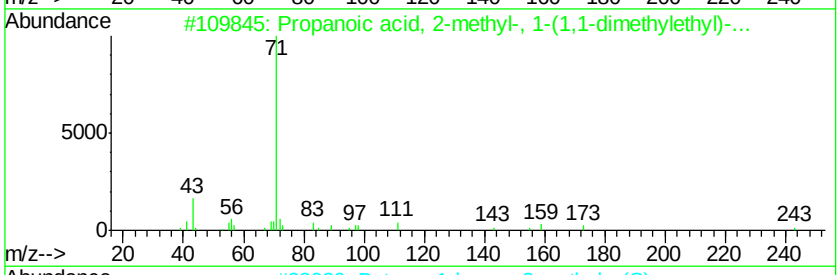
****

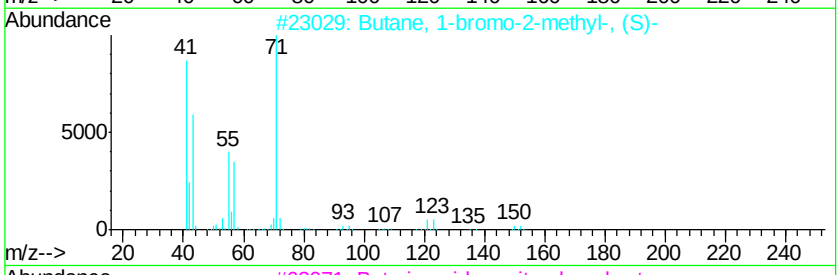
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 7

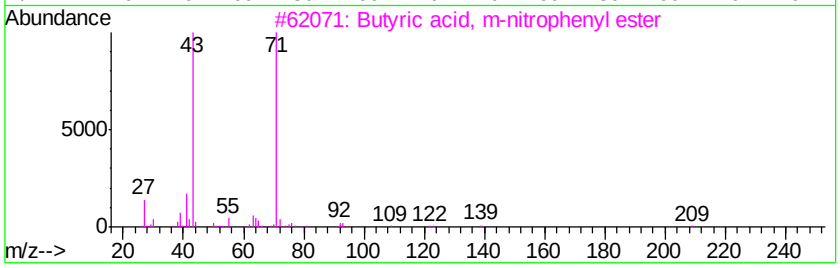
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.19 ng	190447	Acenaphthene-d10	9.85

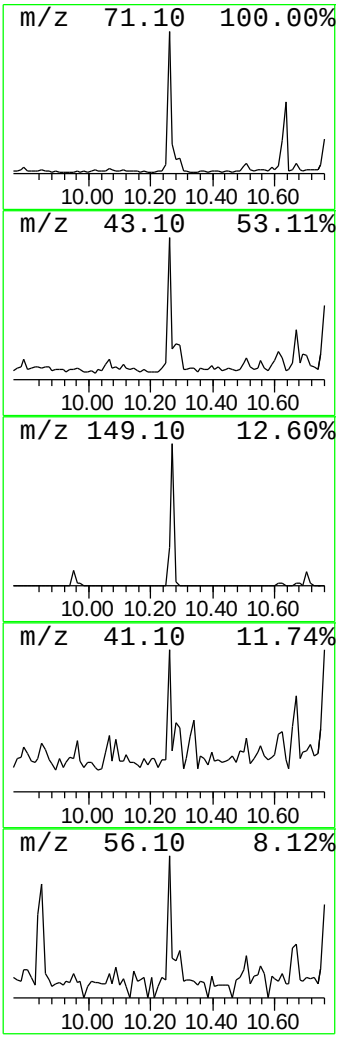
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	64
2	Butane, 1-bromo-2-methyl-, (S)-	150	C5H11Br	000534-00-9	53
3	Butyric acid, m-nitrophenyl ester	209	C10H11NO4	014617-97-1	53
4	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	53
5	Butane, 1-bromo-2-methyl-	150	C5H11Br	010422-35-2	53











Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

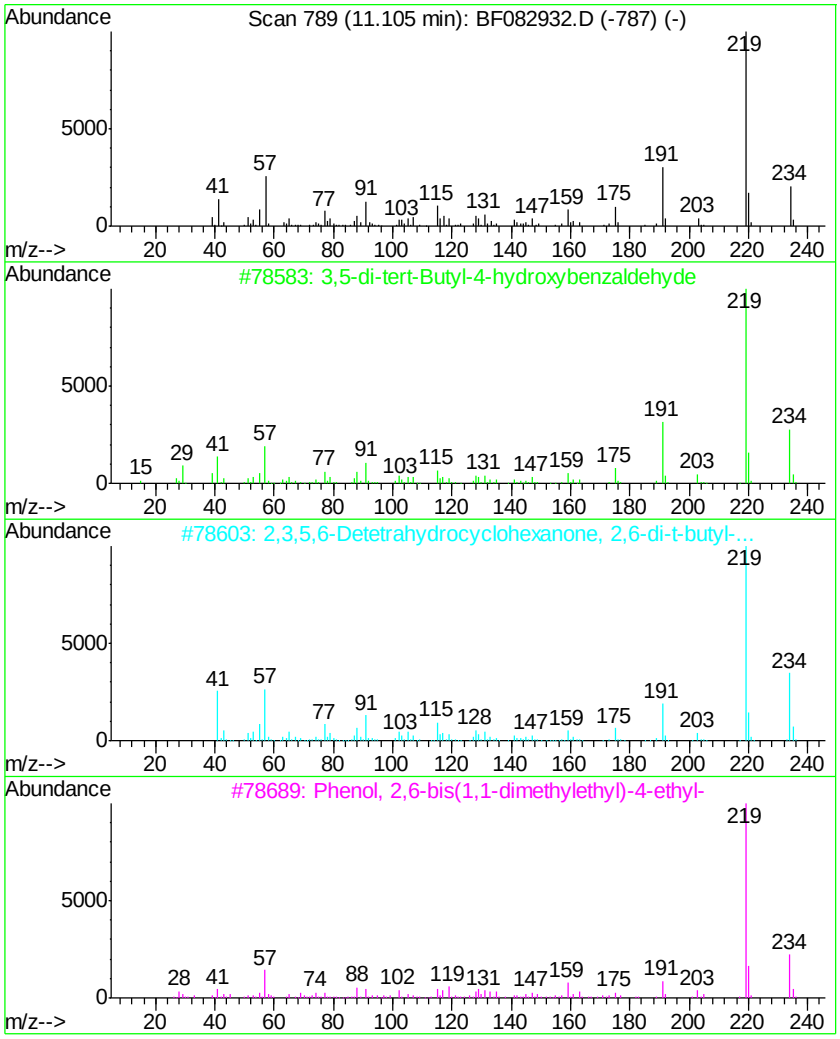
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

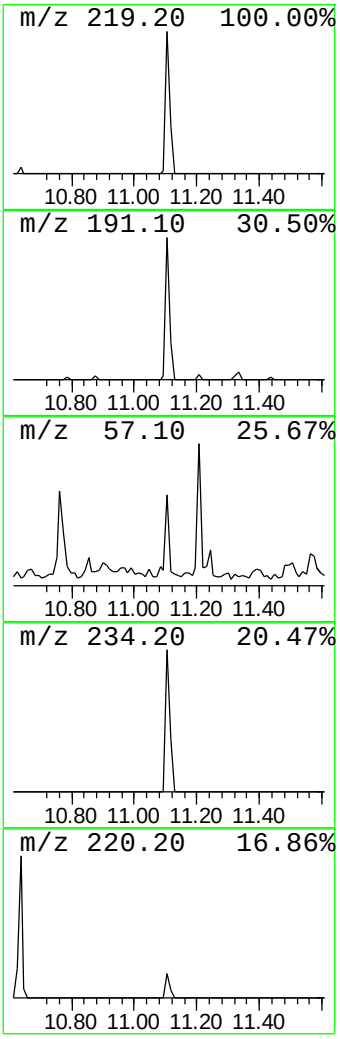
****

Peak Number 7 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.11	2.50 ng	184643	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	98
2	2,3,5,6-Detetrahydrocyclohexanon...	234	C15H22O2	101100-38-3	97
3	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	81
4	6-Tert.butyl-2,3-dicyanonaphthalen	234	C16H14N2	032703-82-5	80
5	4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

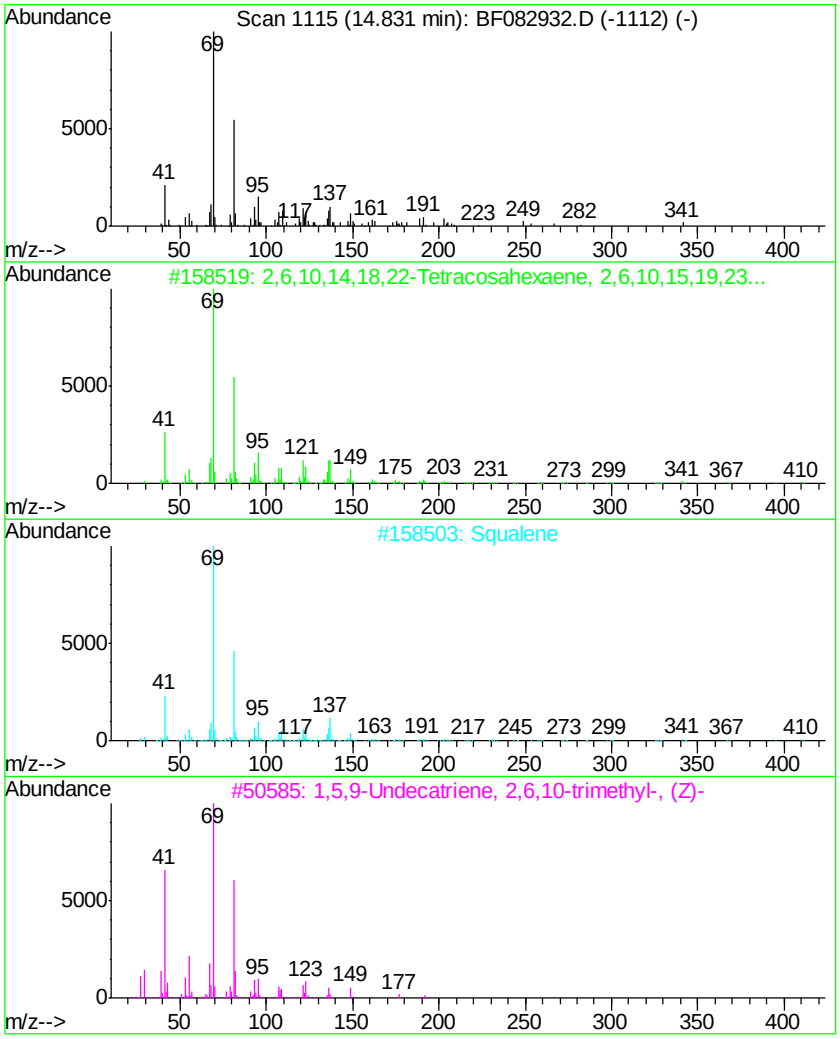
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

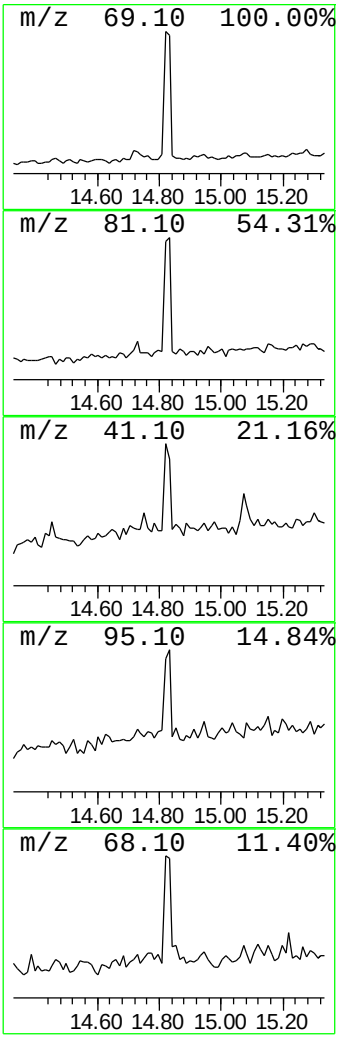
****

Peak Number 8 2,6,10,14,18,22-Tetracosahe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.02 ng	110919	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
2	Squalene	410	C30H50	007683-64-9	80
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	59





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Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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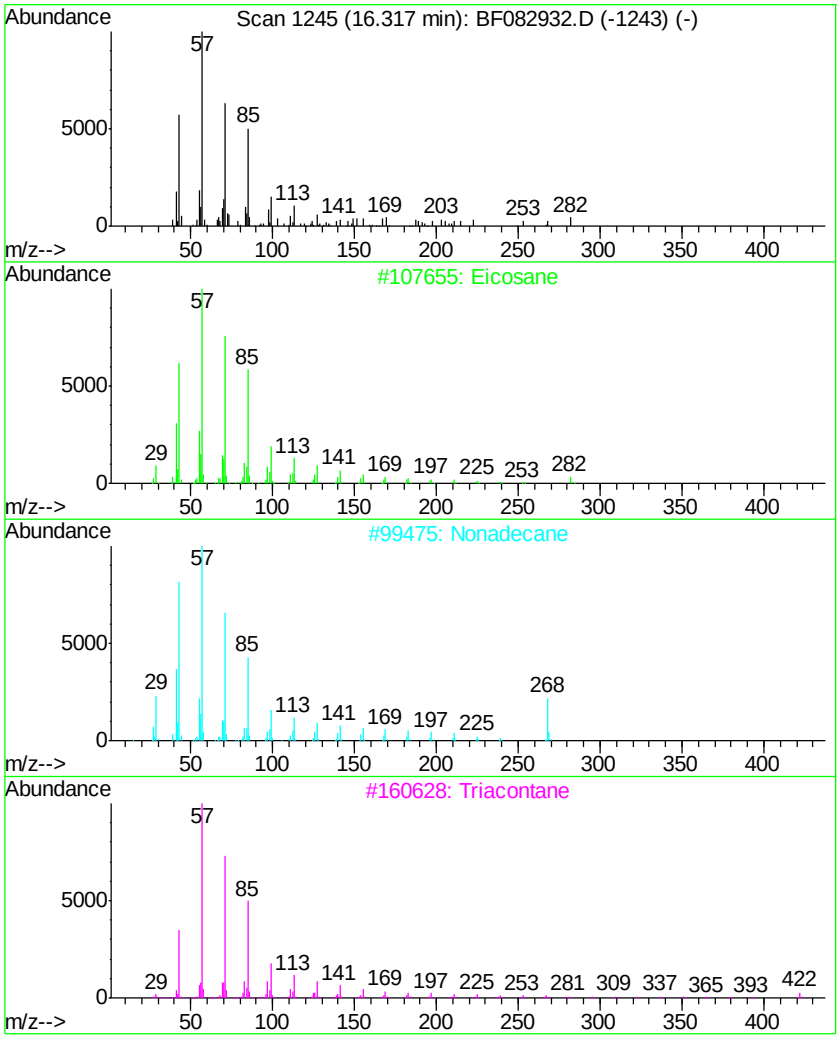
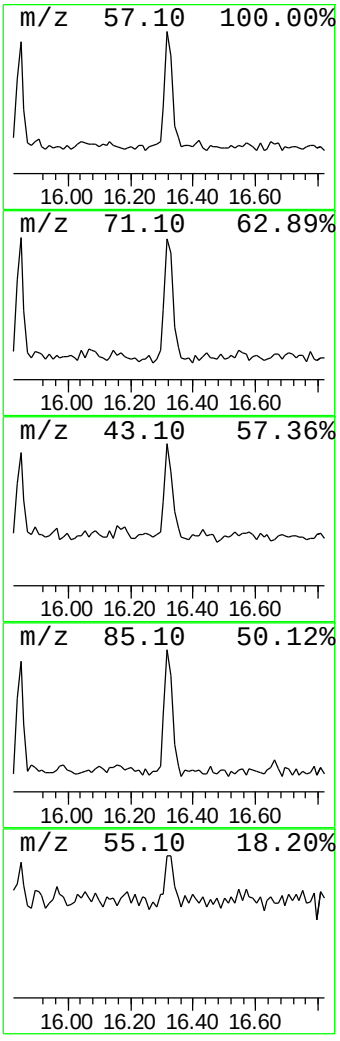
Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.05 ng	112512	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Nonadecane	268	C19H40	000629-92-5	87
3	Triacontane	422	C30H62	000638-68-6	80
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	80
5	Docosane	310	C22H46	000629-97-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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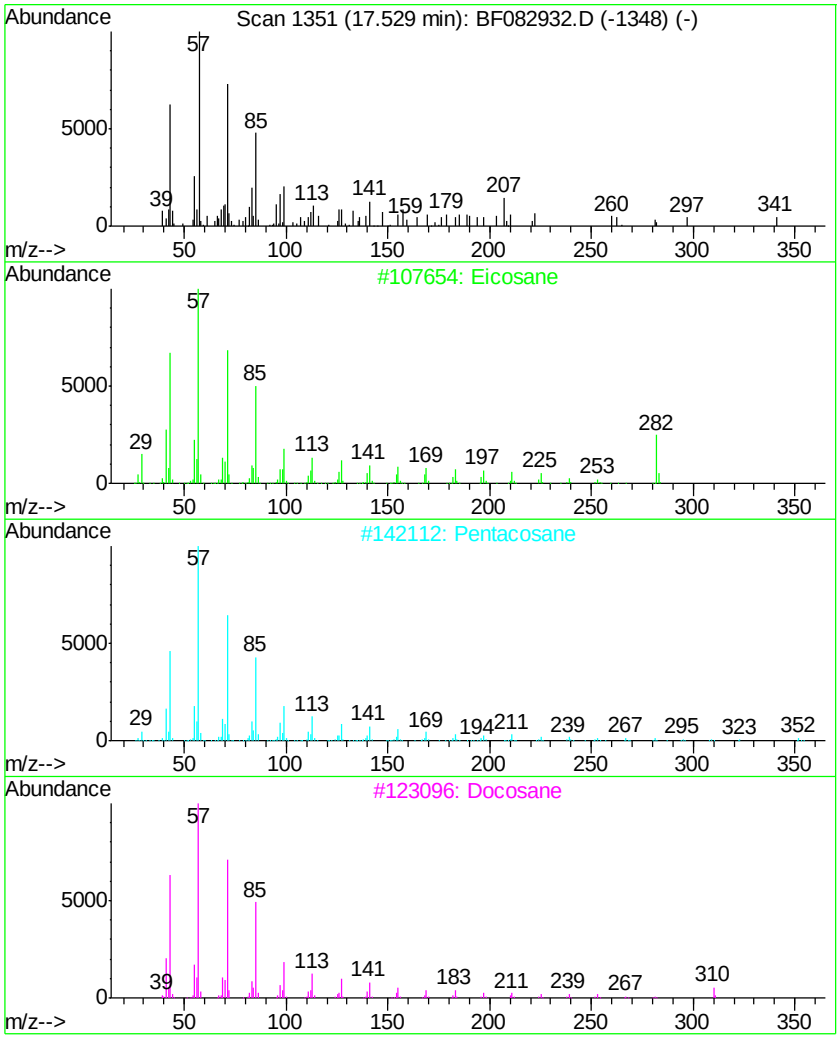
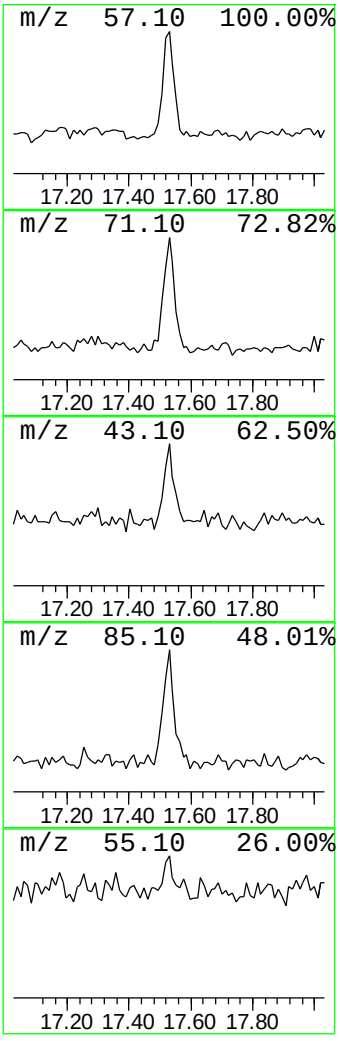
Peak Number 10 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.53	2.21 ng	121307	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	70
2	Pentacosane	352	C25H52	000629-99-2	62
3	Docosane	310	C22H46	000629-97-0	62
4	Hexacosane	366	C26H54	000630-01-3	62
5	Octadecane, 1,1'-[(1-methyl-1,2-...	581	C39H80O2	035545-51-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082932.D
Acq On : 14 Nov 2015 9:08
Operator : UM/IZ
Sample : G4331-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-002-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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
2-Pentanone, 4-hy...	4.97	15.4	ng	913503	1	6.81	1183750	20.0
unknown6.58	6.58	77.6	ng	4595500	1	6.81	1183750	20.0
Benzene, 1-ethyl-...	7.84	2.2	ng	183632	2	8.09	1642240	20.0
Naphthalene, 2,3-...	9.50	2.1	ng	182439	3	9.85	1739540	20.0
Propanoic acid, 2...	10.26	2.2	ng	190447	3	9.85	1739540	20.0
3,5-di-tert-Butyl...	11.11	2.5	ng	184643	4	11.32	1475650	20.0
2,6,10,14,18,22-T...	14.83	2.0	ng	110919	6	15.39	1098470	20.0
Eicosane	16.32	2.0	ng	112512	6	15.39	1098470	20.0
Pentacosane	17.53	2.2	ng	121307	6	15.39	1098470	20.0