LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083857.D
Acq On : 16 Dec 2015 19:25
Operator : UM/SJ
Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

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-BF121315.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	2.167	5	7	16	rVB	27622	59039	2.24%	0.275%
2	5.081	259	262	268	rBV	409753	509192	19.28%	2.368%
3	5.504	296	299	301	rBV	1860017	1872923	70.91%	8.711%
4	6.522	385	388	391	rBV	1437590	1810485	68.55%	8.421%
5	6.659	397	400	403	rVB	1979084	1829427	69.26%	8.509%
6	6.887	418	420	423	rBV	561676	499867	18.93%	2.325%
7	7.047	432	434	436	rBV	1819195	1550099	58.69%	7.210%
8	7.447	466	469	472	rBV	1010840	1201741	45.50%	5.589%
9	8.179	530	533	535	rBV	480575	661961	25.06%	3.079%
10	9.253	624	627	629	rBV	2742592	2641304	100.00%	12.285%
11	9.642	659	661	663	rBV	510222	419610	15.89%	1.952%
12	9.802	672	675	676	rBV2	19149	29454	1.12%	0.137%
13	9.848	676	679	683	rVB2	31212	77490	2.93%	0.360%
14	9.928	683	686	688	rBV	939330	841689	31.87%	3.915%
15	10.248	713	714	717	rVB2	18122	27145	1.03%	0.126%
16	10.339	720	722	723	rBV2	35355	31629	1.20%	0.147%
17	10.362	723	724	726	rVB	77365	65074	2.46%	0.303%
18	10.591	740	744	746	rBV	38911	65844	2.49%	0.306%
19	10.716	752	755	757	rBV	1395174	1482741	56.14%	6.896%
20	10.842	761	766	770	rBV2	87622	193125	7.31%	0.898%
21	10.933	770	774	775	rBV3	21955	45907	1.74%	0.214%
22	11.048	780	784	789	rVV7	30676	97867	3.71%	0.455%
23	11.162	792	794	797	rVB3	16464	29378	1.11%	0.137%
24	11.288	803	805	806	rVV	52825	46952	1.78%	0.218%
25	11.311	806	807	811	rVB2	37951	51501	1.95%	0.240%
26	11.402	813	815	819	rBV	545241	845032	31.99%	3.930%
27	11.482	819	822	823	rVB2	28892	49190	1.86%	0.229%
28	11.905	858	859	861	rBV	16727	31566	1.20%	0.147%
29	12.019	867	869	874	rVB3	44856	82020	3.11%	0.381%
30	12.236	886	888	890	rVB2	20267	29369	1.11%	0.137%
31	12.454	905	907	909	rBV2	37835	51093	1.93%	0.238%
32	12.499	909	911	913	rVB3	19227	32597	1.23%	0.152%
33	12.614	919	921	923	rBV	178255	176617	6.69%	0.821%
34	12.842	938	941	945	rBV	182861	205963	7.80%	0.958%

LSC Area Percent Report

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Data File : BF083857.D
Acq On : 16 Dec 2015 19:25
Operator : UM/SJ
Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.991	952	954	957	rBV	2147620	2080241	78.76%	9.676%
36	13.151	966	968	969	rBV	28709	36789	1.39%	0.171%
37	13.277	977	979	983	rVB2	25842	43643	1.65%	0.203%
38	13.471	994	996	998	rVB	35364	33976	1.29%	0.158%
39	13.677	1013	1014	1019	rVB	24916	41710	1.58%	0.194%
40	13.779	1021	1023	1025	rBV3	13415	27498	1.04%	0.128%
41	13.882	1030	1032	1036	rBV	77355	103669	3.92%	0.482%
42	13.962	1037	1039	1041	rVB	25832	28264	1.07%	0.131%
43	14.042	1043	1046	1047	rBV	560451	638119	24.16%	2.968%
44	14.522	1086	1088	1089	rBV2	19351	29983	1.14%	0.139%
45	15.060	1133	1135	1140	rVB	49421	98178	3.72%	0.457%
46	15.357	1158	1161	1163	rBV	36441	47957	1.82%	0.223%
47	15.414	1164	1166	1169	rVB	42543	51873	1.96%	0.241%
48	15.482	1169	1172	1174	rBV	303248	460317	17.43%	2.141%
49	16.168	1230	1232	1238	rVB6	17565	41367	1.57%	0.192%
50	16.900	1293	1296	1301	rVB2	21886	52204	1.98%	0.243%
51	17.323	1330	1333	1337	rVB	17184	39332	1.49%	0.183%

Sum of corrected areas: 21500011

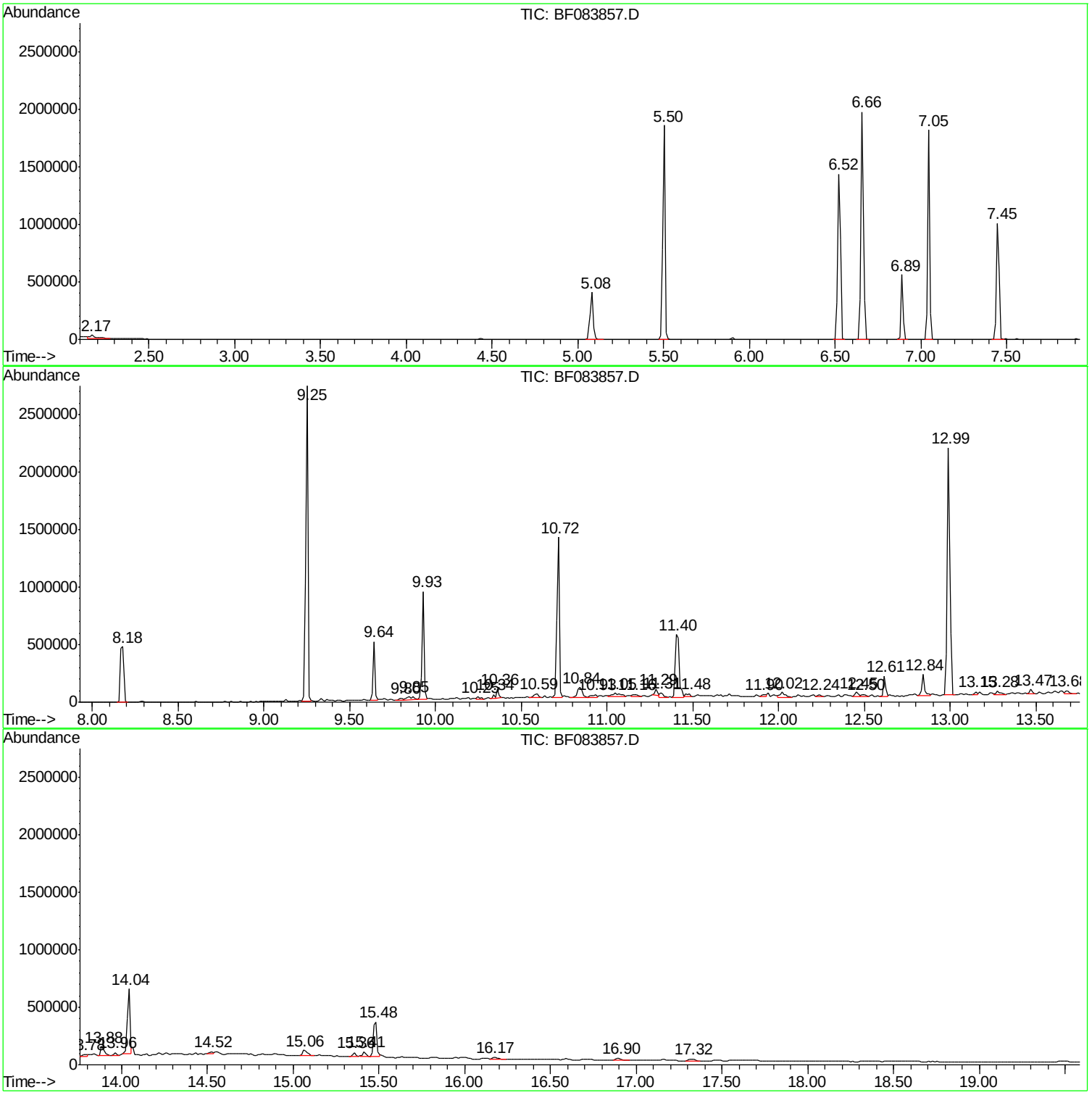
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083857.D
Acq On : 16 Dec 2015 19:25
Operator : UM/SJ
Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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\BF121615\
Data File : BF083857.D
Acq On : 16 Dec 2015 19:25
Operator : UM/SJ
Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

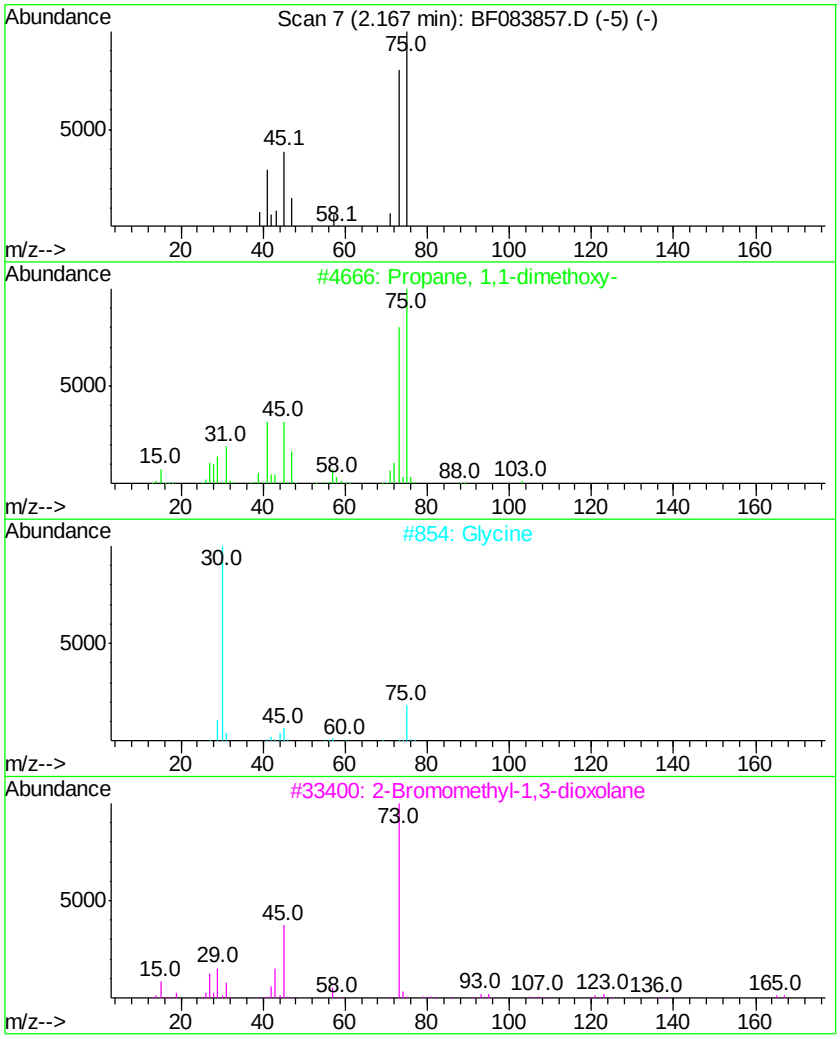
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

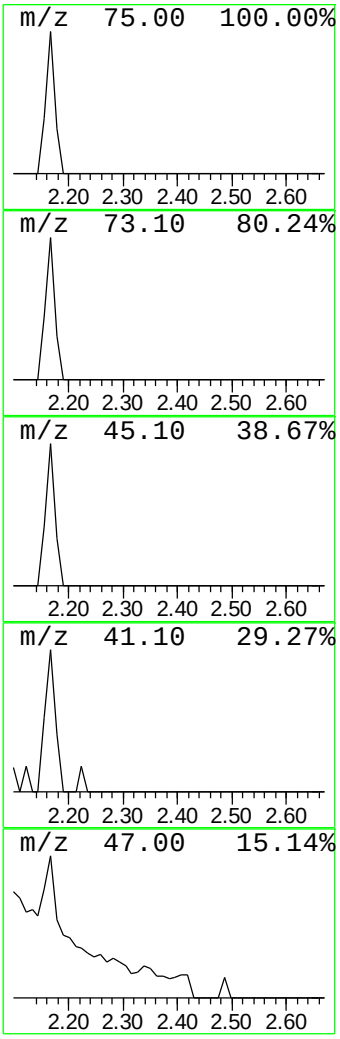
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.36 ng	59039	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Glycine	75	C2H5NO2	000056-40-6	5
3	2-Bromomethyl-1,3-dioxolane	166	C4H7BrO2	004360-63-8	4
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	4
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083857.D
Acq On : 16 Dec 2015 19:25
Operator : UM/SJ
Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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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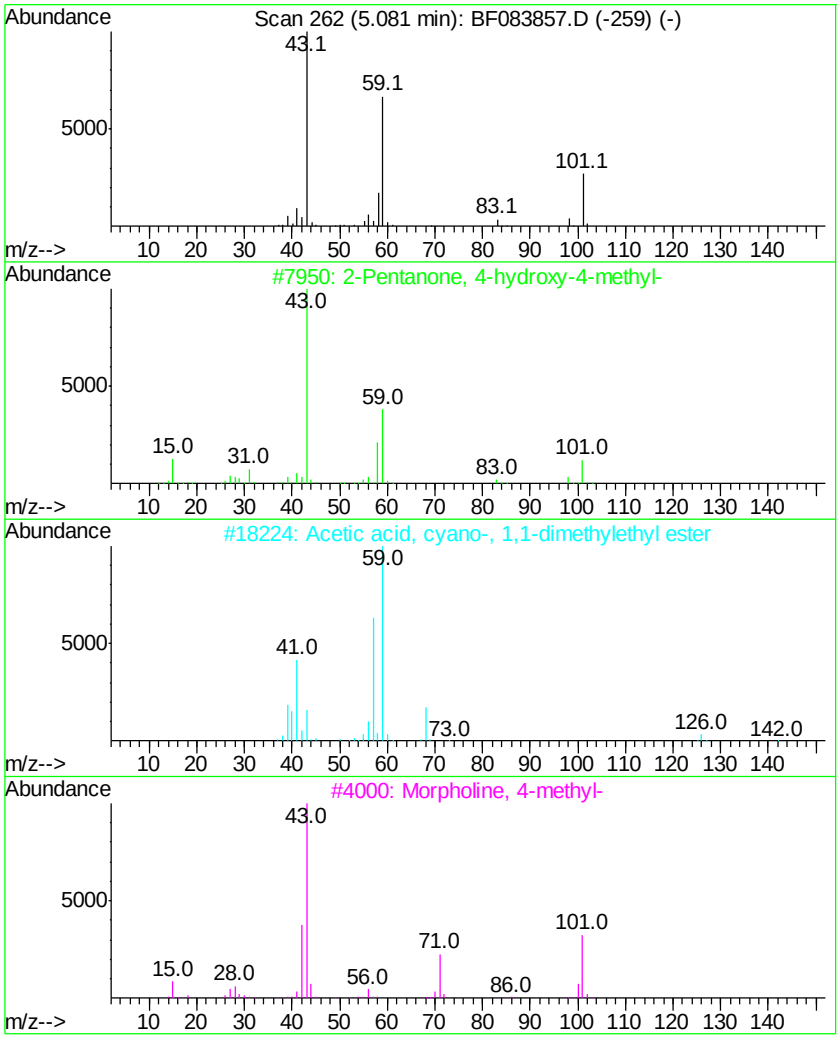
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	20.37 ng	509192	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



m/z 43.10 100.00%
m/z 59.10 66.68%
m/z 101.10 26.96%
m/z 58.10 17.06%
m/z 41.10 9.34%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083857.D
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Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

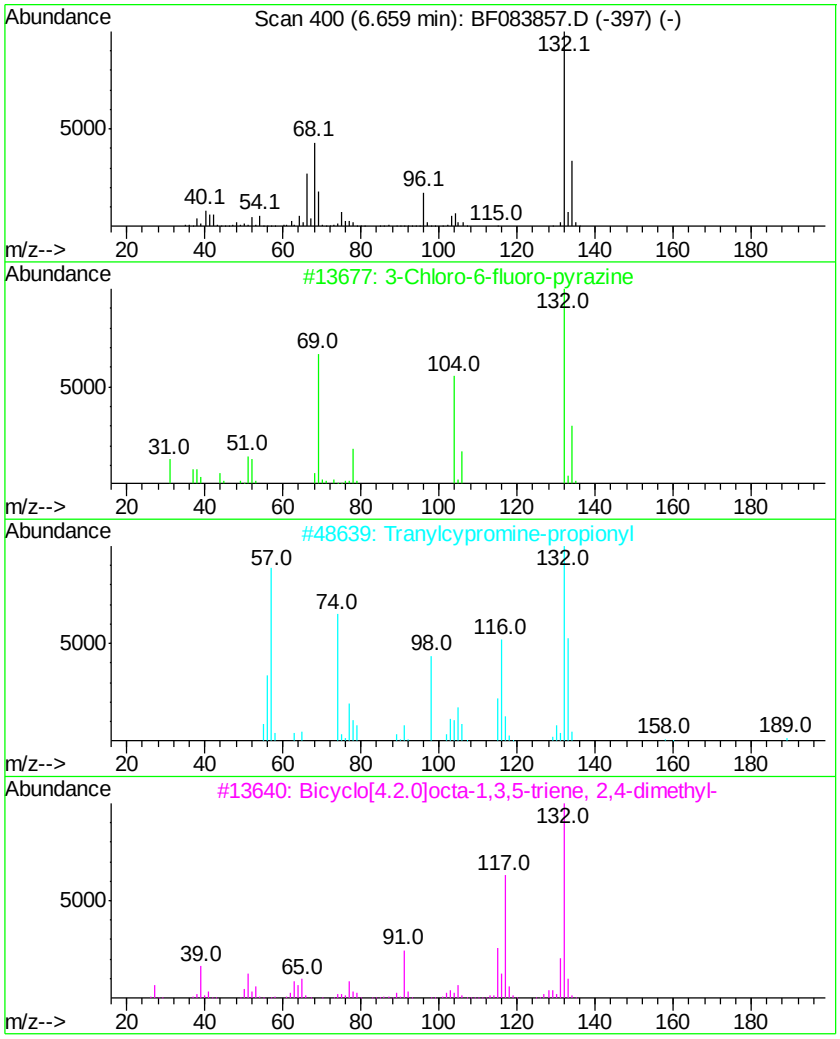
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

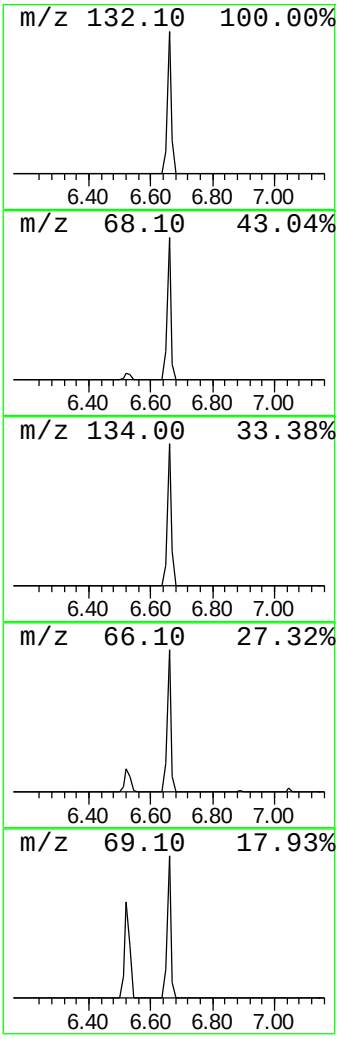
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	73.20 ng	1829430	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
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Acq On : 16 Dec 2015 19:25
Operator : UM/SJ
Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

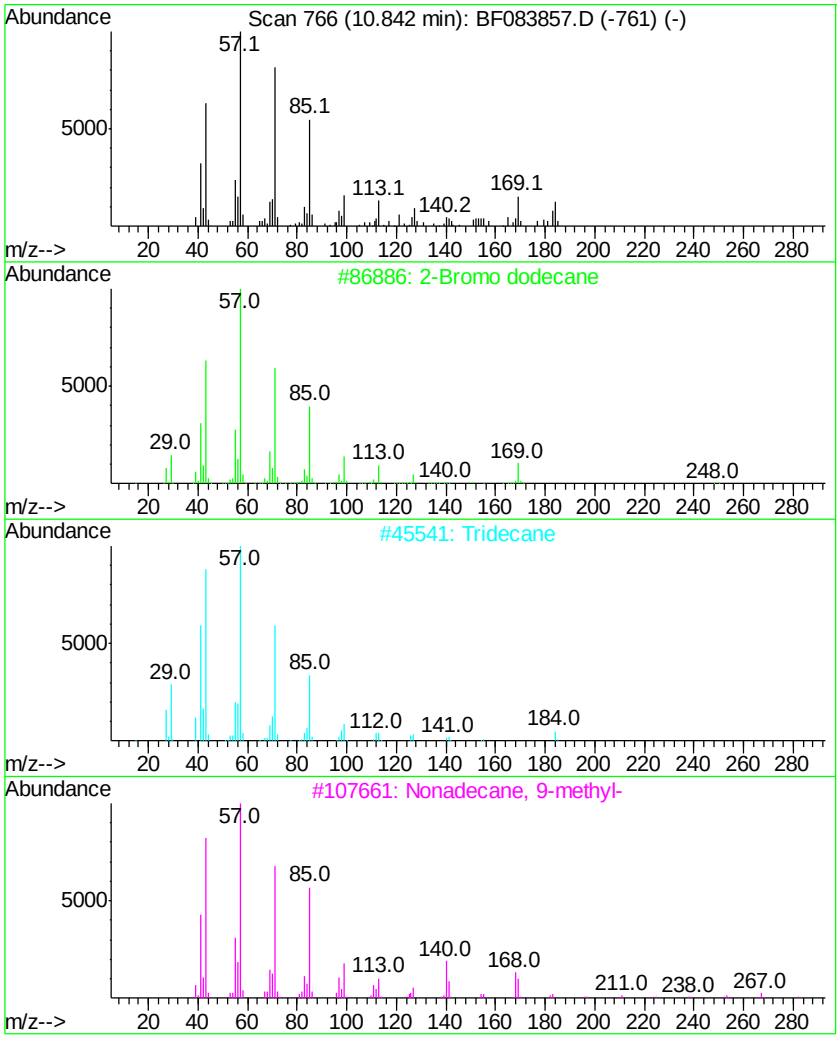
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

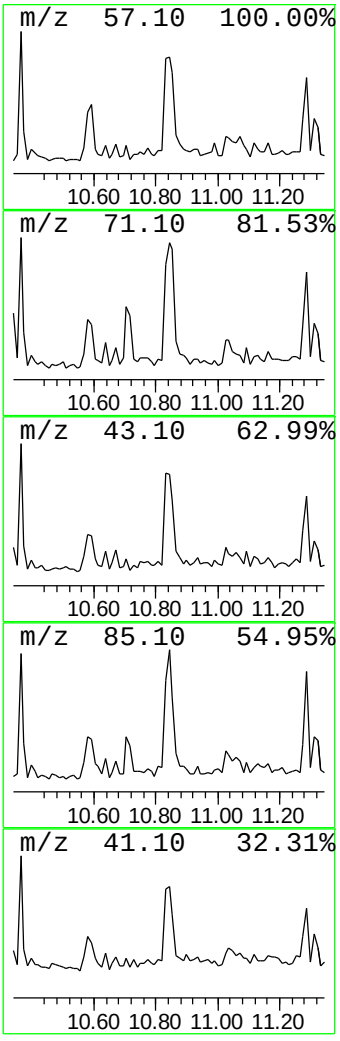
****

Peak Number 5 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	4.57 ng	193125	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	87
2	Tridecane	184	C13H28	000629-50-5	87
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
4	Octadecane	254	C18H38	000593-45-3	83
5	Heptadecane	240	C17H36	000629-78-7	83





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Data File : BF083857.D
Acq On : 16 Dec 2015 19:25
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Sample : G4836-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

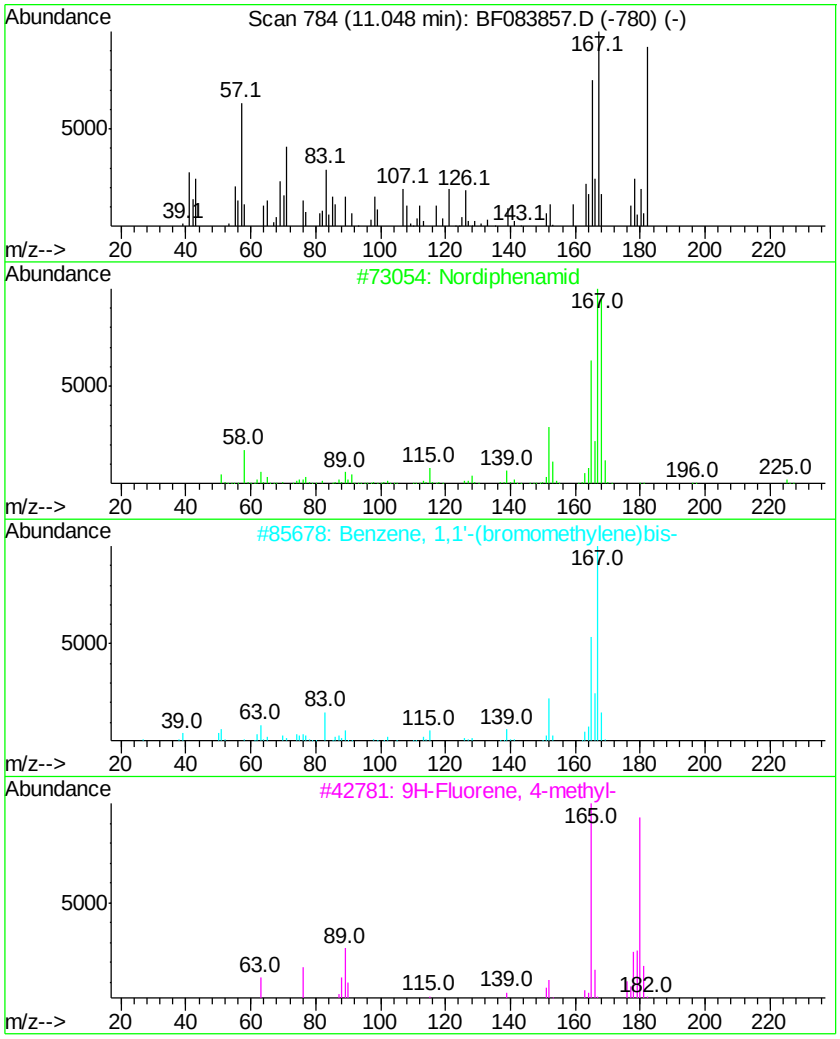
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

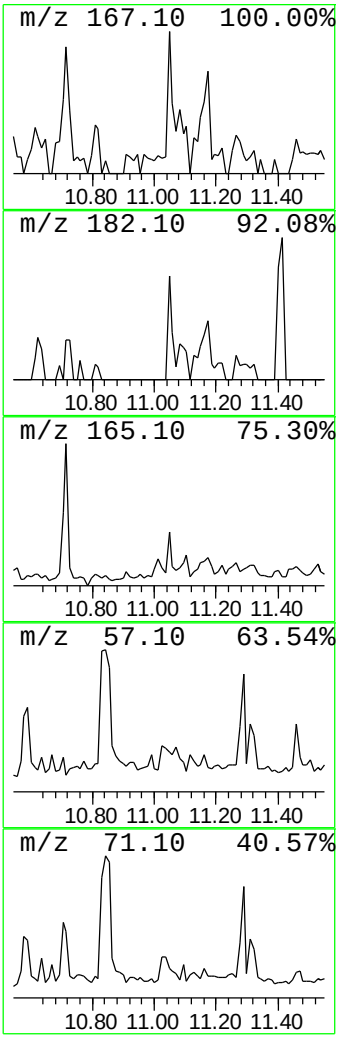
****

Peak Number 6 unknown11.05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	2.32 ng	97867	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nordiphenamid	225	C15H15NO	000954-21-2	25
2	Benzene, 1,1'-(bromomethylene)bis-	246	C13H11Br	000776-74-9	25
3	9H-Fluorene, 4-methyl-	180	C14H12	001556-99-6	18
4	9H-Fluorene, 2-methyl-	180	C14H12	001430-97-3	15
5	Benzene, 1,1'-(chloromethylene)bis-	202	C13H11Cl	000090-99-3	12





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Sample : G4836-05
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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY-SF-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

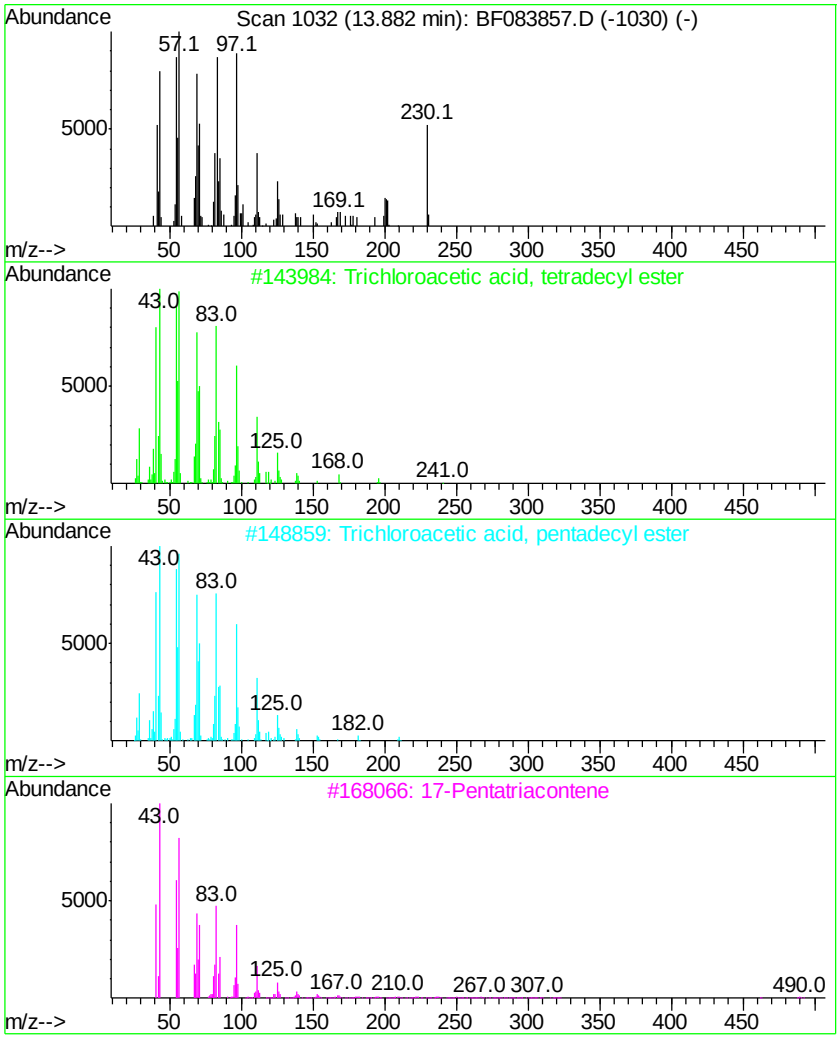
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

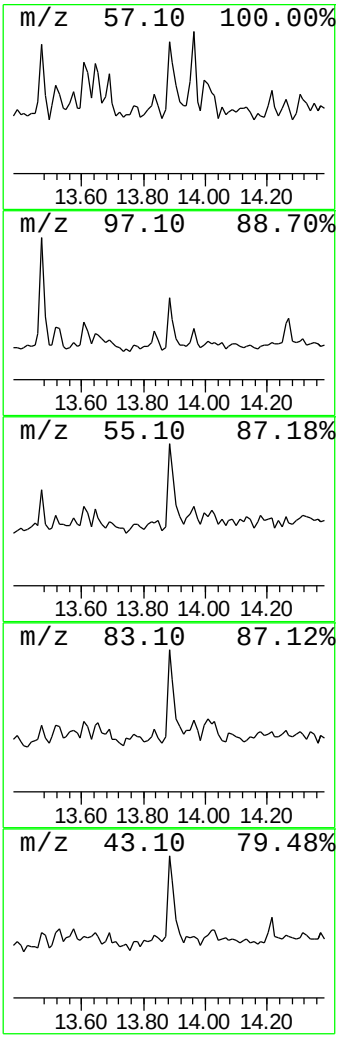
****

Peak Number 7 Trichloroacetic acid, tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.25 ng	103669	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	80
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	64
3	17-Pentatriacontene	491	C35H70	006971-40-0	64
4	1-Heptadecanol	256	C17H36O	001454-85-9	58
5	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121615\
Data File : BF083857.D
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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
Propane, 1,1-dime...	2.17	2.4	ng	59039	1	6.89	499867	20.0
2-Pentanone, 4-hy...	5.08	20.4	ng	509192	1	6.89	499867	20.0
unknown6.66	6.66	73.2	ng	1829430	1	6.89	499867	20.0
2-Bromo dodecane	10.84	4.6	ng	193125	4	11.41	845032	20.0
unknown11.05	11.05	2.3	ng	97867	4	11.41	845032	20.0
Trichloroacetic a...	13.88	3.3	ng	103669	5	14.04	638119	20.0