LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

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-BF123115.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	20	rVB	68297	149270	1.75%	0.239%
2	3.870	150	156	159	rBV	125235	194530	2.27%	0.312%
3	5.082	259	262	268	rVB	629377	795663	9.30%	1.275%
4	5.504	296	299	301	rBV	4467051	4459041	52.13%	7.146%
5	6.533	386	389	391	rBV	2144357	2787911	32.59%	4.468%
6	6.659	397	400	403	rBV	6294165	6422285	75.09%	10.292%
7	6.887	418	420	422	rBV	2154443	1781031	20.82%	2.854%
8	7.047	431	434	436	rVB	7065482	6343013	74.16%	10.165%
9	7.459	467	470	472	rVB	5368757	5920585	69.22%	9.488%
10	7.802	497	500	501	rBV	356877	302690	3.54%	0.485%
11	7.825	501	502	505	rVV	270910	279918	3.27%	0.449%
12	7.916	508	510	513	rBV	185175	223949	2.62%	0.359%
13	8.179	530	533	535	rBV	2287635	2375866	27.78%	3.807%
14	8.899	593	596	599	rBV	63572	89364	1.04%	0.143%
15	9.253	624	627	630	rBV	8045517	8553247	100.00%	13.707%
16	9.653	660	662	663	rBV	250242	300578	3.51%	0.482%
17	9.859	678	680	684	rBV	82645	109967	1.29%	0.176%
18	9.928	684	686	689	rVB2	2229928	2414530	28.23%	3.869%
19	10.362	721	724	726	rBV2	212612	219119	2.56%	0.351%
20	10.568	740	742	747	rBV2	124126	191094	2.23%	0.306%
21	10.716	753	755	758	rBV2	3870836	5579044	65.23%	8.941%
22	10.842	764	766	770	rVB	142006	254745	2.98%	0.408%
23	10.979	775	778	779	rBV	138425	126263	1.48%	0.202%
24	11.288	802	805	806	rBV	121051	120453	1.41%	0.193%
25	11.414	814	816	819	rBV	2575582	2246247	26.26%	3.600%
26	11.631	833	835	837	rBV	183735	192786	2.25%	0.309%
27	12.328	894	896	899	rVB	100537	108966	1.27%	0.175%
28	12.785	934	936	938	rBV	155395	169235	1.98%	0.271%
29	13.002	952	955	958	rBV	5914586	6199899	72.49%	9.936%
30	13.791	1021	1024	1026	rBV	79247	106936	1.25%	0.171%
31	13.905	1031	1034	1040	rBV	236105	354307	4.14%	0.568%
32	14.054	1044	1047	1049	rBV	1401513	1573129	18.39%	2.521%
33	15.494	1170	1173	1175	rBV	1049957	1454379	17.00%	2.331%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 62400040

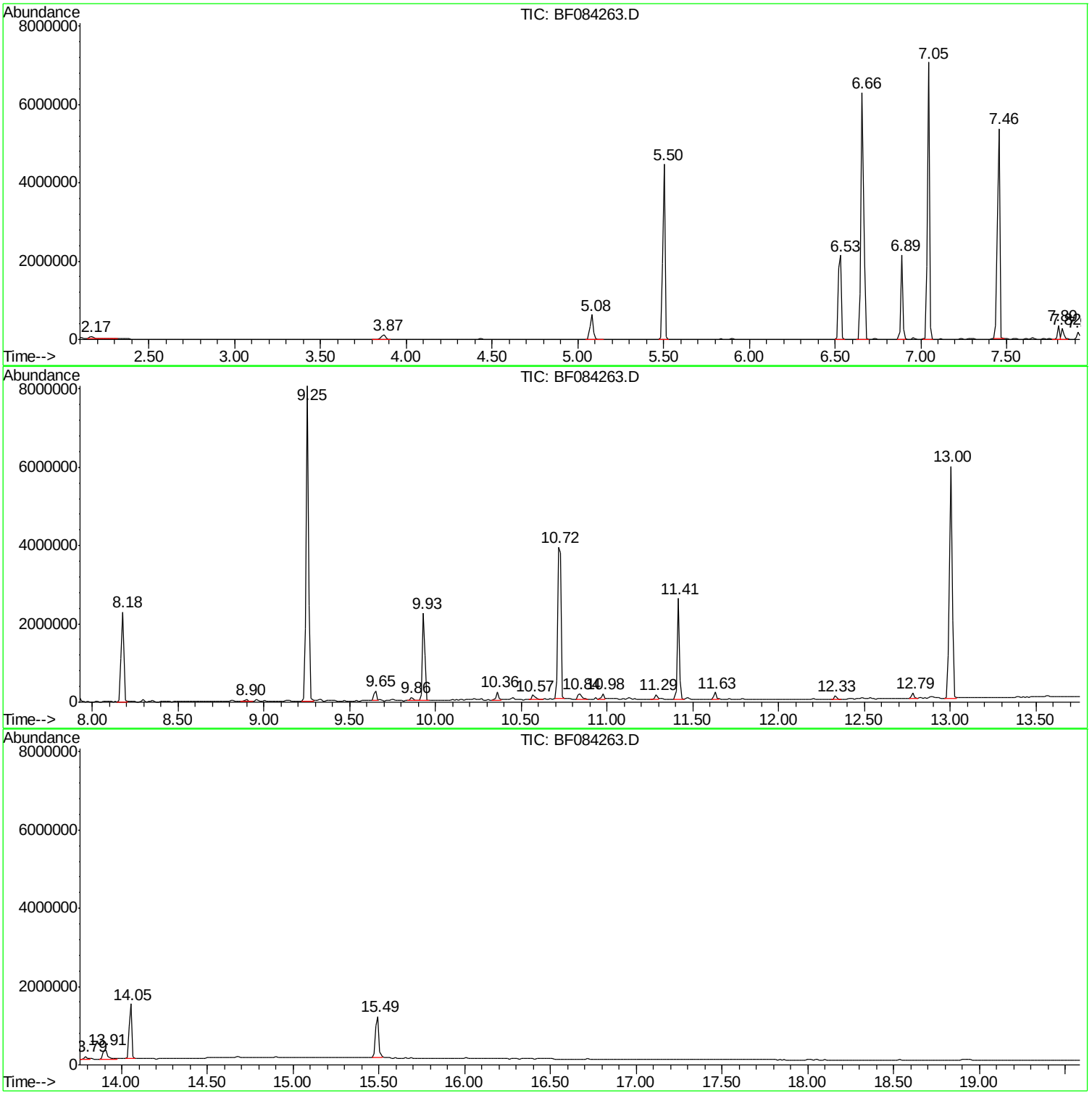
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

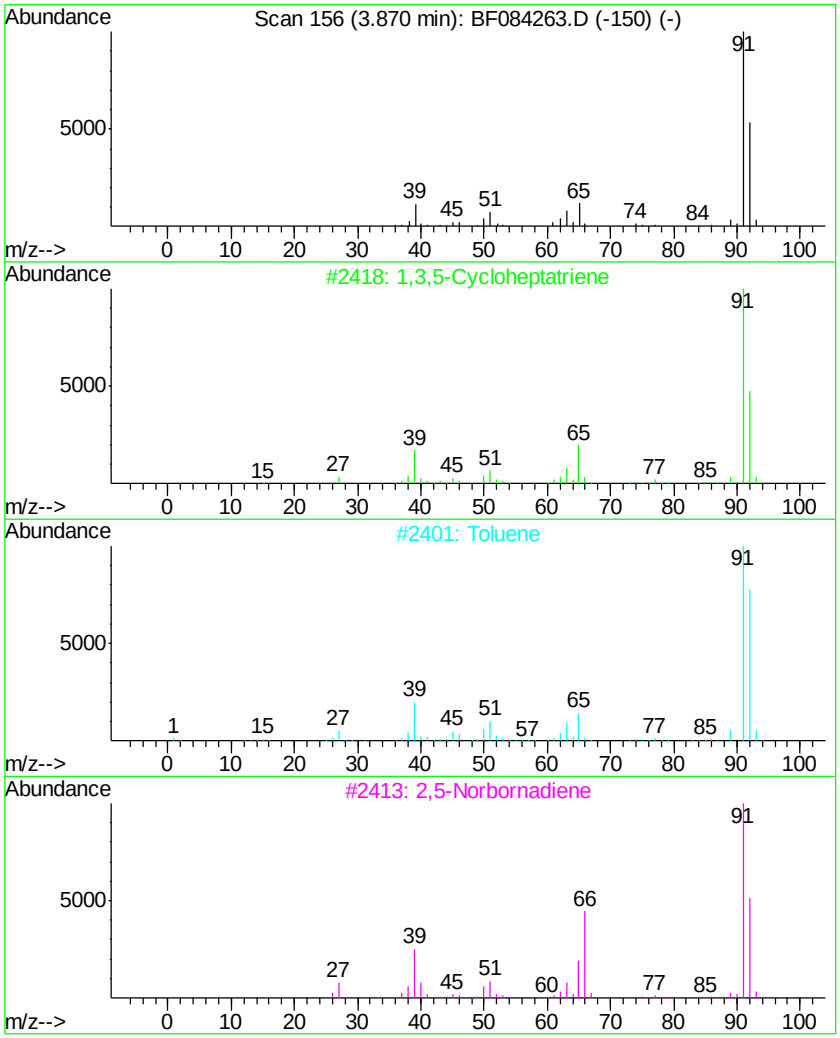
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

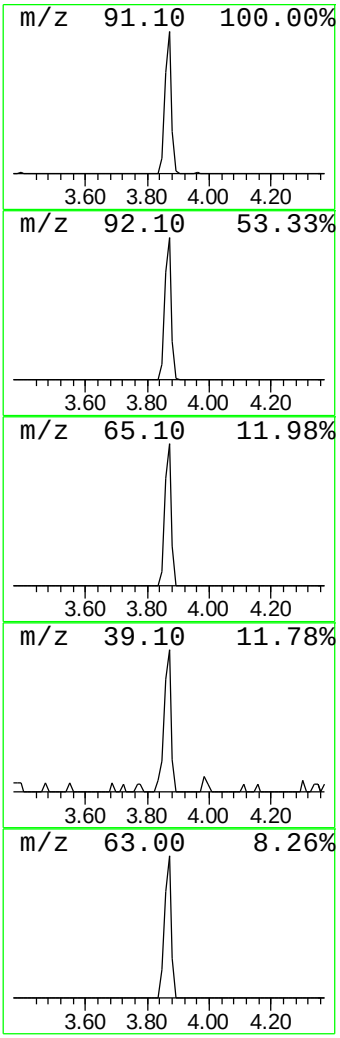
****

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.87	2.18 ng	194530	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	91
2	Toluene	92	C7H8	000108-88-3	87
3	2,5-Norbornadiene	92	C7H8	000121-46-0	80
4	Spiro[2.4]hepta-4,6-diene	92	C7H8	000765-46-8	74
5	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

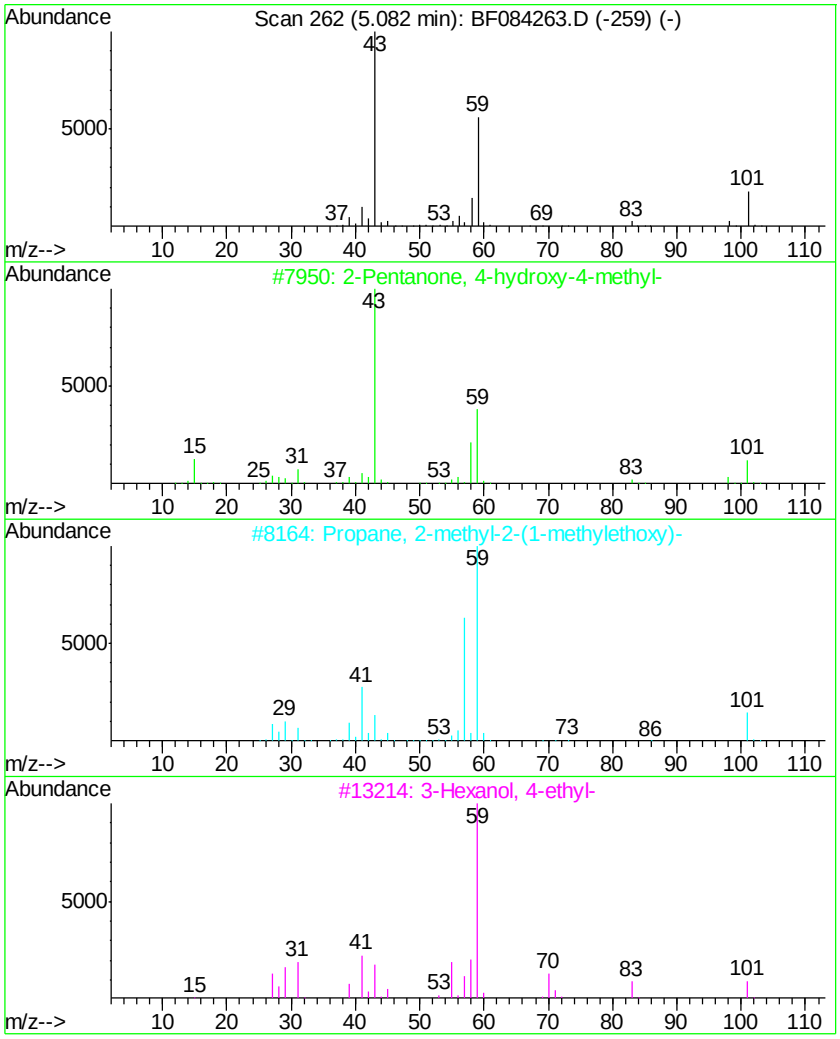
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

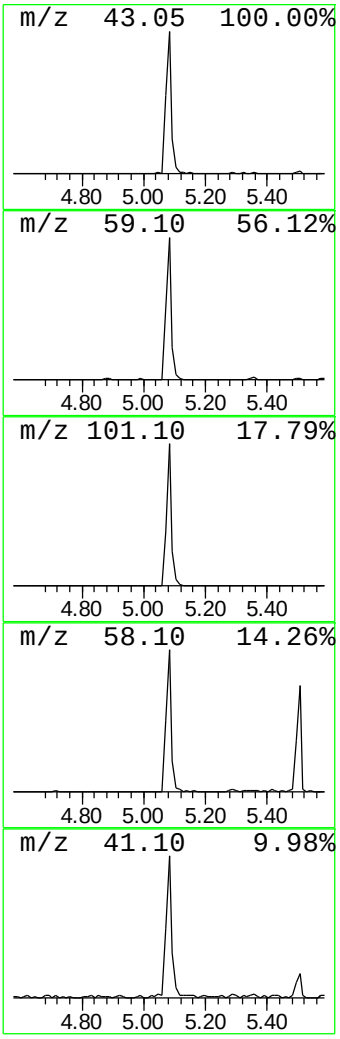
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	8.93 ng	795663	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

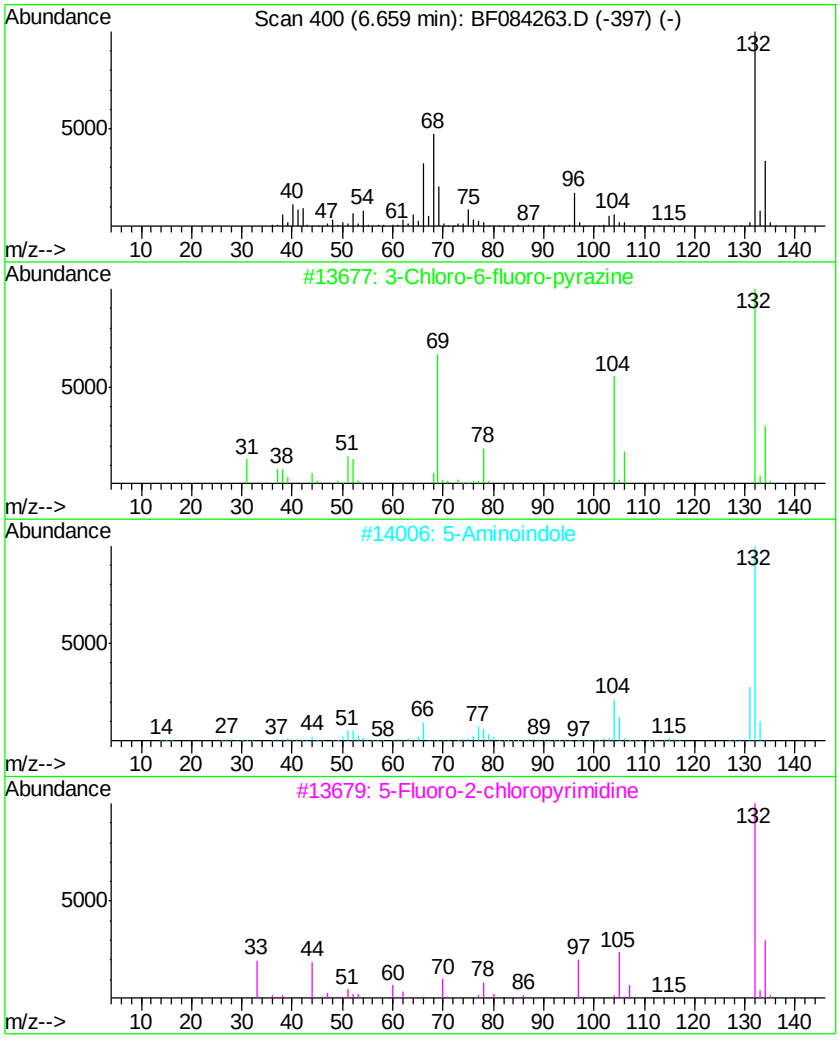
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

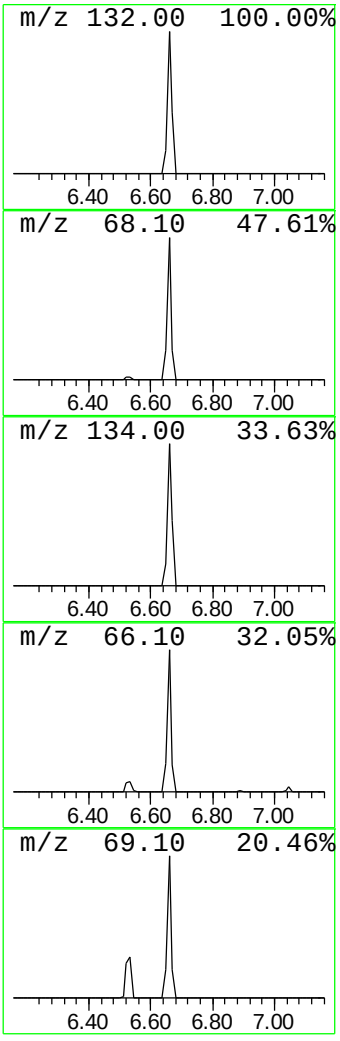
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	72.12 ng	6422290	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	5-Aminoindole	132	C8H8N2	005192-03-0	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





Library Search Compound Report

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Operator : UM/SJ
Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

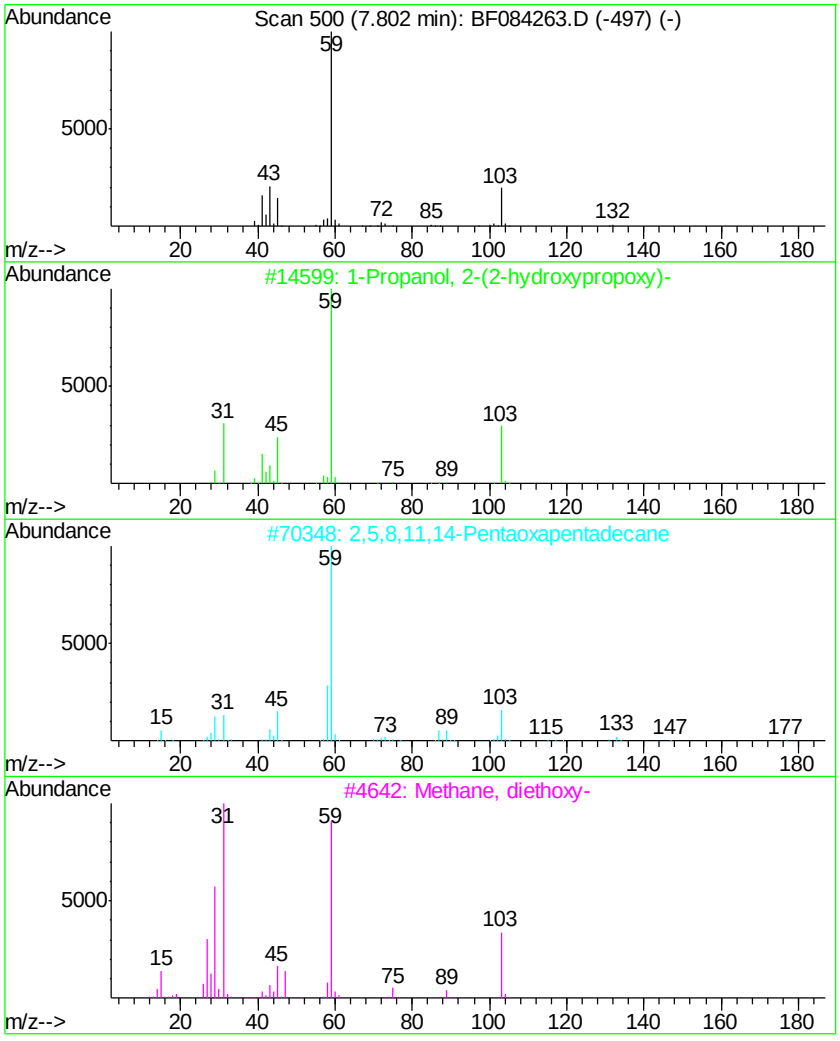
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

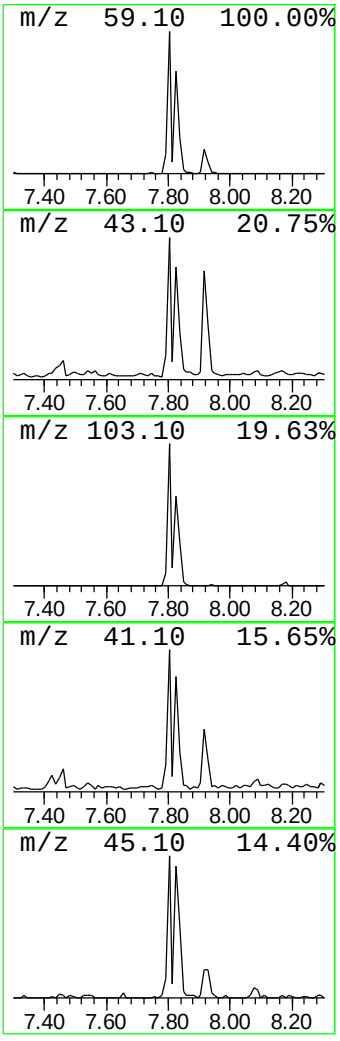
****

Peak Number 5 1-Propanol, 2-(2-hydroxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	2.55 ng	302690	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	83
2	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	78
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	78
4	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	78
5	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	74





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Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

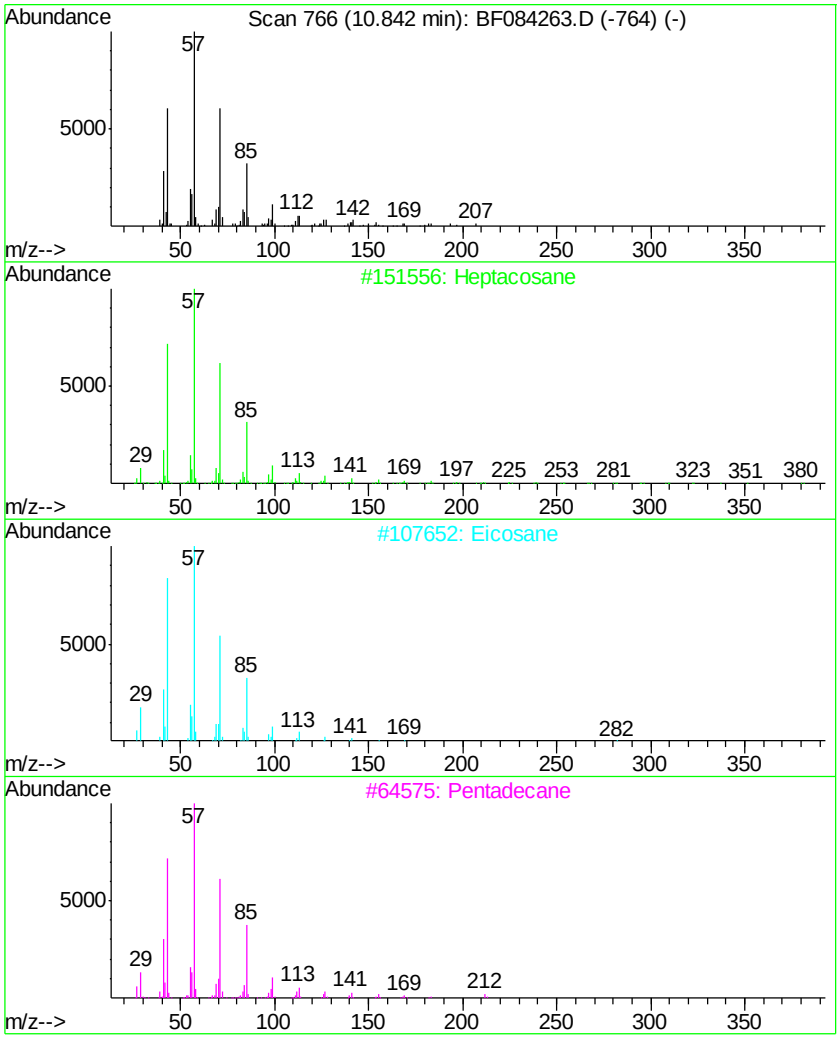
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

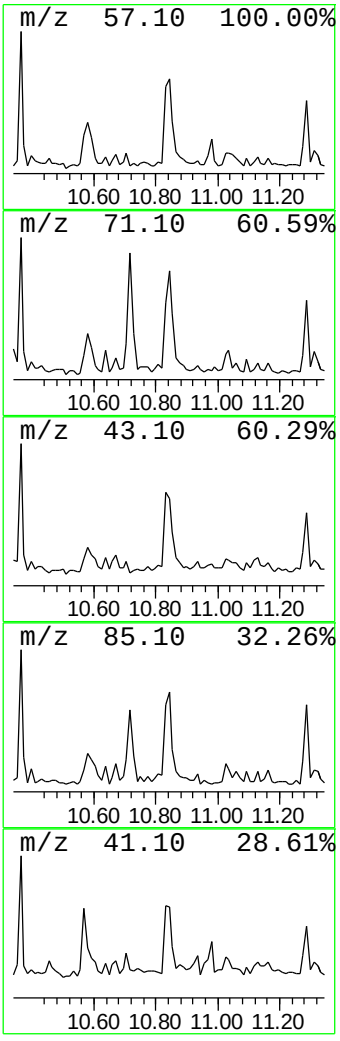
****

Peak Number 7 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.27 ng	254745	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Eicosane	282	C20H42	000112-95-8	87
3	Pentadecane	212	C15H32	000629-62-9	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Hexadecane	226	C16H34	000544-76-3	80





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Sample : G4990-06
Misc :
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Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

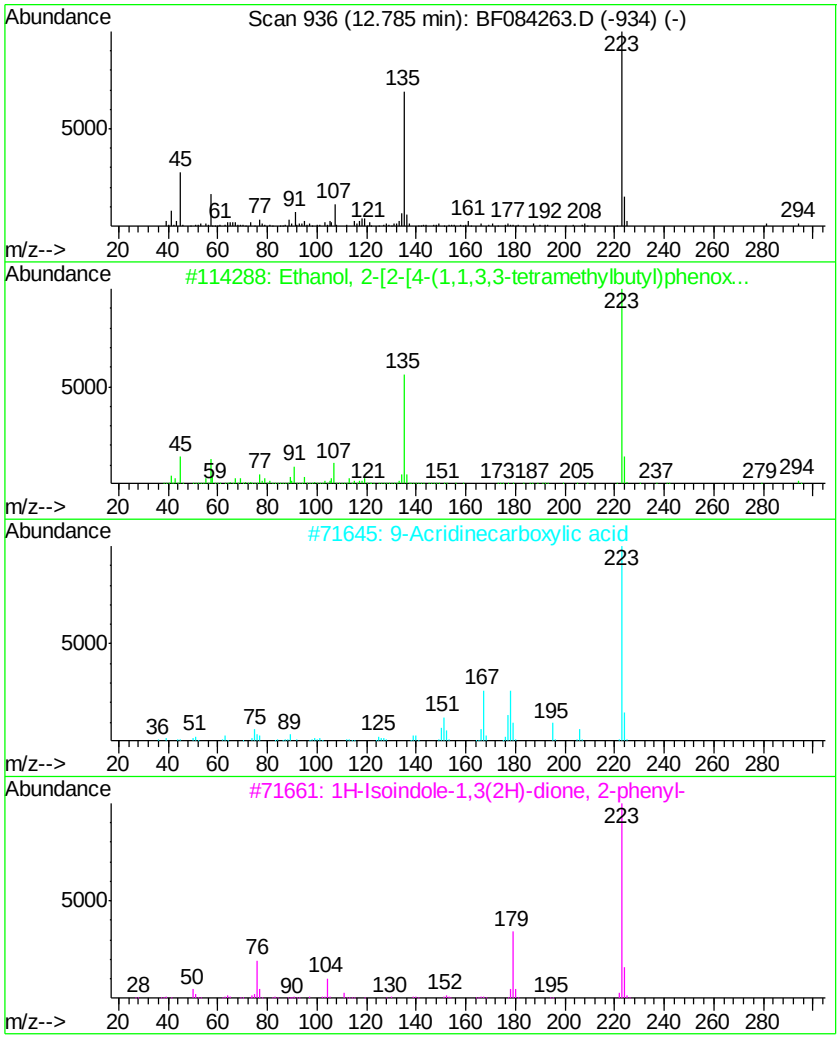
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

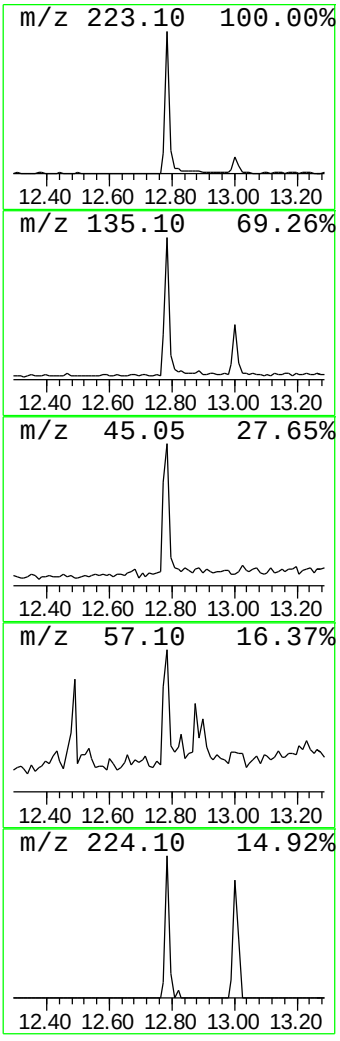
****

Peak Number 8 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.15 ng	169235	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	87
2	9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	32
3	1H-Isoindole-1,3(2H)-dione, 2-ph...	223	C14H9NO2	000520-03-6	32
4	Tetrazole, 1-(4-fluorophenyl)-5-...	400	C23H21FN6	125038-07-5	25
5	2-Propen-1-one, 1-(4-aminophenyl...	223	C15H13NO	002403-30-7	14





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Sample : G4990-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

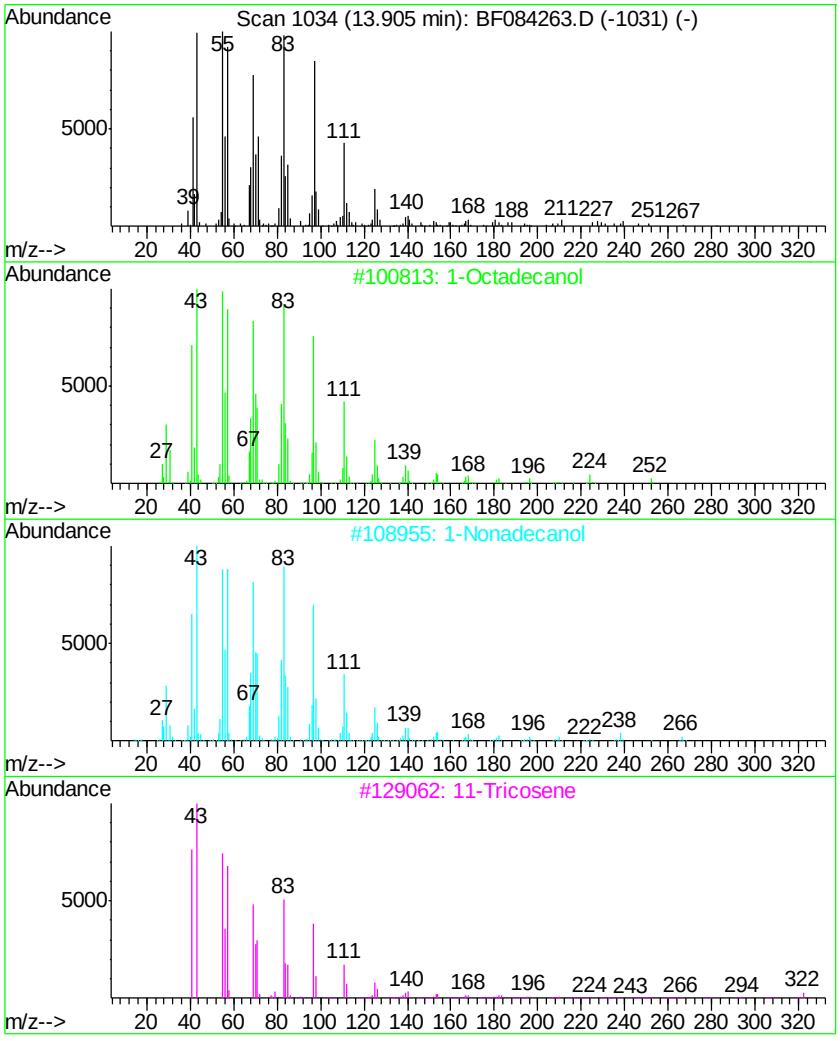
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

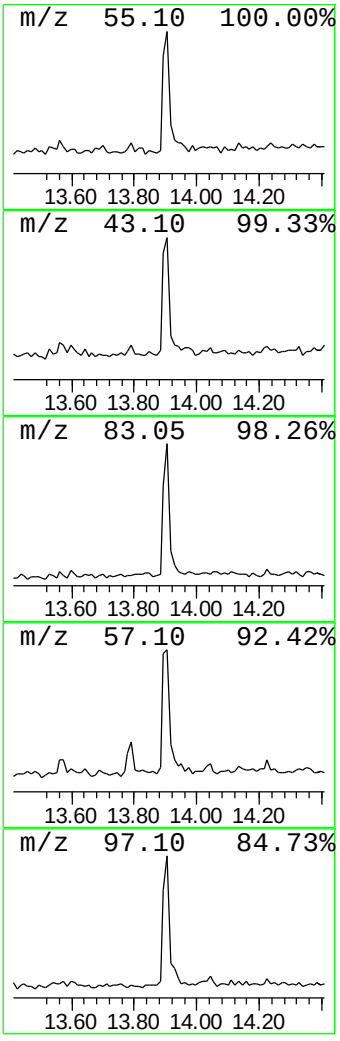
****

Peak Number 9 1-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	4.50 ng	354307	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	94
2	1-Nonadecanol	284	C19H40O	001454-84-8	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084263.D
Acq On : 5 Jan 2016 4:08
Operator : UM/SJ
Sample : G4990-06
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Instrument : BNA_F
ClientSampleId : W-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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
1,3,5-Cycloheptat...	3.87	2.2	ng	194530	1	6.89	1781030	20.0
2-Pentanone, 4-hy...	5.08	8.9	ng	795663	1	6.89	1781030	20.0
unknown6.66	6.66	72.1	ng	6422290	1	6.89	1781030	20.0
1-Propanol, 2-(2-...	7.80	2.5	ng	302690	2	8.18	2375870	20.0
Heptacosane	10.84	2.3	ng	254745	4	11.41	2246250	20.0
Ethanol, 2-[2-[4-...	12.79	2.1	ng	169235	5	14.05	1573130	20.0
1-Octadecanol	13.91	4.5	ng	354307	5	14.05	1573130	20.0