LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

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-BF112115.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	4.787	242	245	253	rVB	1761395	2706580	43.31%	4.054%
2	5.244	283	285	288	rBV	3588472	5163296	82.61%	7.733%
3	6.307	375	378	381	rBV	3864678	6249950	100.00%	9.361%
4	6.421	385	388	390	rBV	4524138	5464784	87.44%	8.185%
5	6.639	405	407	410	rBV	1667471	1456477	23.30%	2.181%
6	6.730	413	415	417	rBV	303355	293389	4.69%	0.439%
7	6.799	418	421	423	rBV	4641437	4335595	69.37%	6.493%
8	7.210	454	457	460	rBV	3148756	3103044	49.65%	4.647%
9	7.359	466	470	472	rBV	161580	233292	3.73%	0.349%
10	7.702	498	500	509	rBV2	31727	73834	1.18%	0.111%
11	7.930	517	520	522	rBV	2043113	1888339	30.21%	2.828%
12	8.707	586	588	590	rBV	86198	117807	1.88%	0.176%
13	9.016	612	615	617	rBV	3984587	5852737	93.64%	8.766%
14	9.405	647	649	656	rBV	889469	1011946	16.19%	1.516%
15	9.542	659	661	663	rVB2	48066	62748	1.00%	0.094%
16	9.679	670	673	675	rBV	1906209	1896881	30.35%	2.841%
17	9.885	688	691	692	rBV	93604	99896	1.60%	0.150%
18	10.102	706	710	711	rBV	37017	74153	1.19%	0.111%
19	10.125	711	712	714	rVV	123047	97627	1.56%	0.146%
20	10.216	718	720	724	rVB	130014	178124	2.85%	0.267%
21	10.342	729	731	733	rBV2	41670	63875	1.02%	0.096%
22	10.468	739	742	744	rBV	1773550	2305173	36.88%	3.452%
23	10.593	751	753	755	rBV	146688	167805	2.68%	0.251%
24	10.639	755	757	760	rVB	194872	230593	3.69%	0.345%
25	10.959	784	785	788	rVB	66810	64950	1.04%	0.097%
26	11.039	791	792	798	rVB2	153219	224100	3.59%	0.336%
27	11.153	799	802	806	rBV2	1637454	2639963	42.24%	3.954%
28	11.222	806	808	810	rVB	301934	337692	5.40%	0.506%
29	11.393	820	823	827	rBV2	105571	208101	3.33%	0.312%
30	11.462	827	829	833	rVV2	67174	110164	1.76%	0.165%
31	11.553	835	837	840	rVB	288882	314100	5.03%	0.470%
32	11.656	844	846	847	rBV	112134	134344	2.15%	0.201%
33	11.702	847	850	851	rVV2	297690	412907	6.61%	0.618%
34	11.759	854	855	860	rVB2	263519	360620	5.77%	0.540%

LSC Area Percent Report

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Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

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-BF112115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.953	869	872	877	rVB2	88387	197285	3.16%	0.295%
36	12.125	886	887	891	rVB3	30892	68735	1.10%	0.103%
37	12.193	891	893	895	rBV2	76136	140292	2.24%	0.210%
38	12.239	895	897	900	rVB2	35582	69517	1.11%	0.104%
39	12.285	900	901	905	rVB2	84846	86883	1.39%	0.130%
40	12.353	905	907	910	rBV	1342739	1514589	24.23%	2.268%
41	12.479	917	918	922	rBV3	84483	202706	3.24%	0.304%
42	12.582	922	927	930	rBV2	1379880	1795047	28.72%	2.688%
43	12.639	930	932	936	rVB3	57517	110269	1.76%	0.165%
44	12.742	938	941	943	rVB	3539263	4155727	66.49%	6.224%
45	12.811	943	947	948	rBV2	86074	111467	1.78%	0.167%
46	12.914	952	956	958	rBV2	215375	309080	4.95%	0.463%
47	12.982	959	962	963	rBV	152700	163727	2.62%	0.245%
48	13.016	963	965	969	rBV	153131	184380	2.95%	0.276%
49	13.108	971	973	974	rBV	73916	74740	1.20%	0.112%
50	13.142	974	976	979	rBV3	59179	107435	1.72%	0.161%
51	13.211	980	982	985	rVV2	83214	117720	1.88%	0.176%
52	13.394	996	998	999	rBV2	67751	94566	1.51%	0.142%
53	13.416	999	1000	1003	rVB2	87430	134385	2.15%	0.201%
54	13.474	1003	1005	1007	rBV2	52544	93209	1.49%	0.140%
55	13.531	1007	1010	1011	rBV2	115460	220069	3.52%	0.330%
56	13.656	1017	1021	1023	rVB3	608598	1037398	16.60%	1.554%
57	13.702	1023	1025	1027	rVB2	60209	78578	1.26%	0.118%
58	13.782	1028	1032	1036	rBV2	1367534	2907967	46.53%	4.355%
59	13.885	1038	1041	1043	rBV	148433	247701	3.96%	0.371%
60	14.159	1063	1065	1067	rVB	75190	103345	1.65%	0.155%
61	14.285	1074	1076	1079	rVB4	104641	188142	3.01%	0.282%
62	14.777	1116	1119	1123	rBV	505741	987403	15.80%	1.479%
63	14.868	1125	1127	1129	rVB2	118879	139364	2.23%	0.209%
64	15.028	1139	1141	1144	rVB	262178	374410	5.99%	0.561%
65	15.085	1144	1146	1149	rVV	451088	528832	8.46%	0.792%
66	15.142	1149	1151	1158	rVB	820672	1141762	18.27%	1.710%
67	15.782	1204	1207	1211	rVB	414760	624960	10.00%	0.936%
68	16.400	1258	1261	1266	rVB2	166726	294184	4.71%	0.441%
69	16.777	1291	1294	1297	rBV	104058	227962	3.65%	0.341%

Sum of corrected areas: 66768722

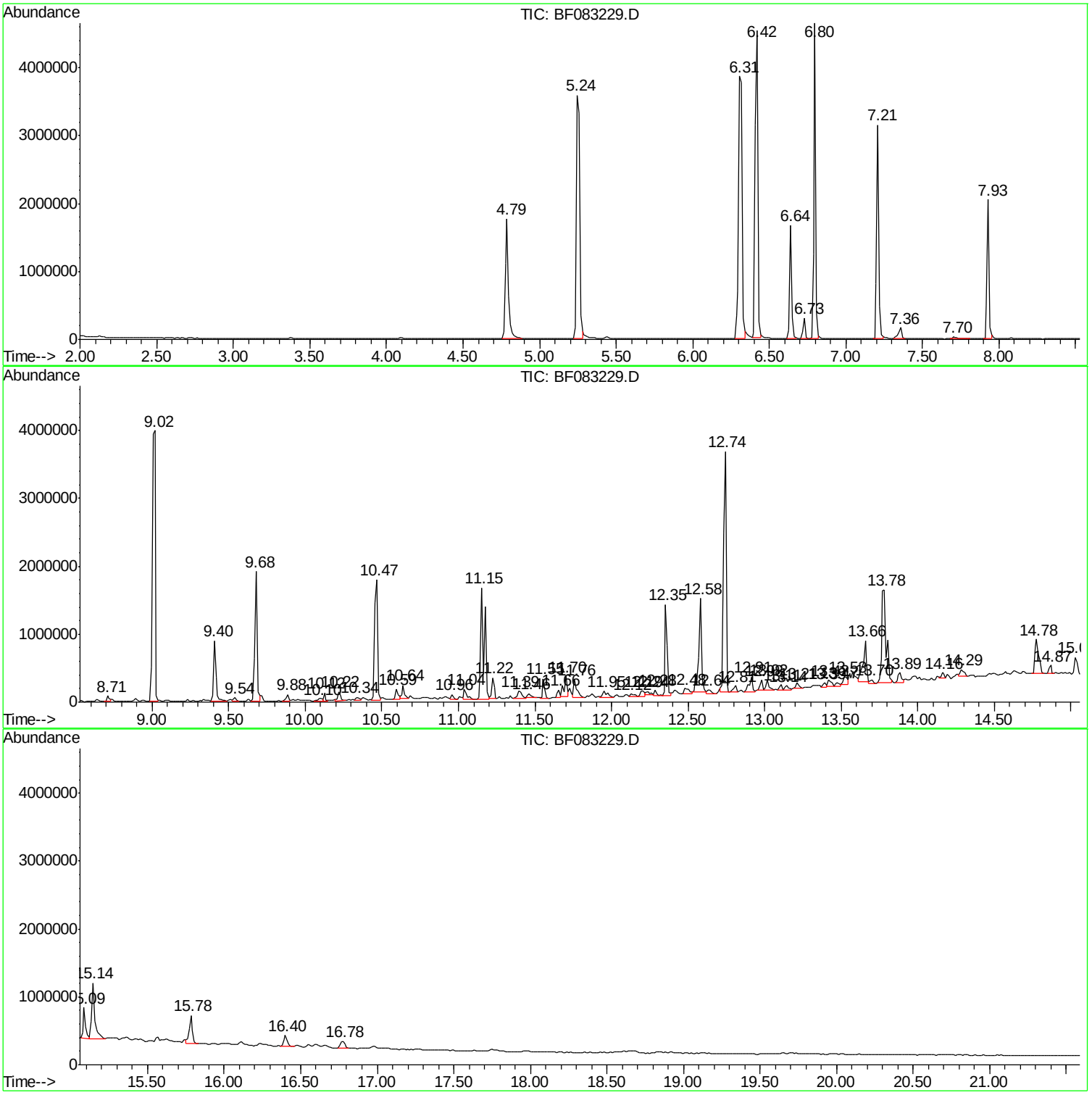
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
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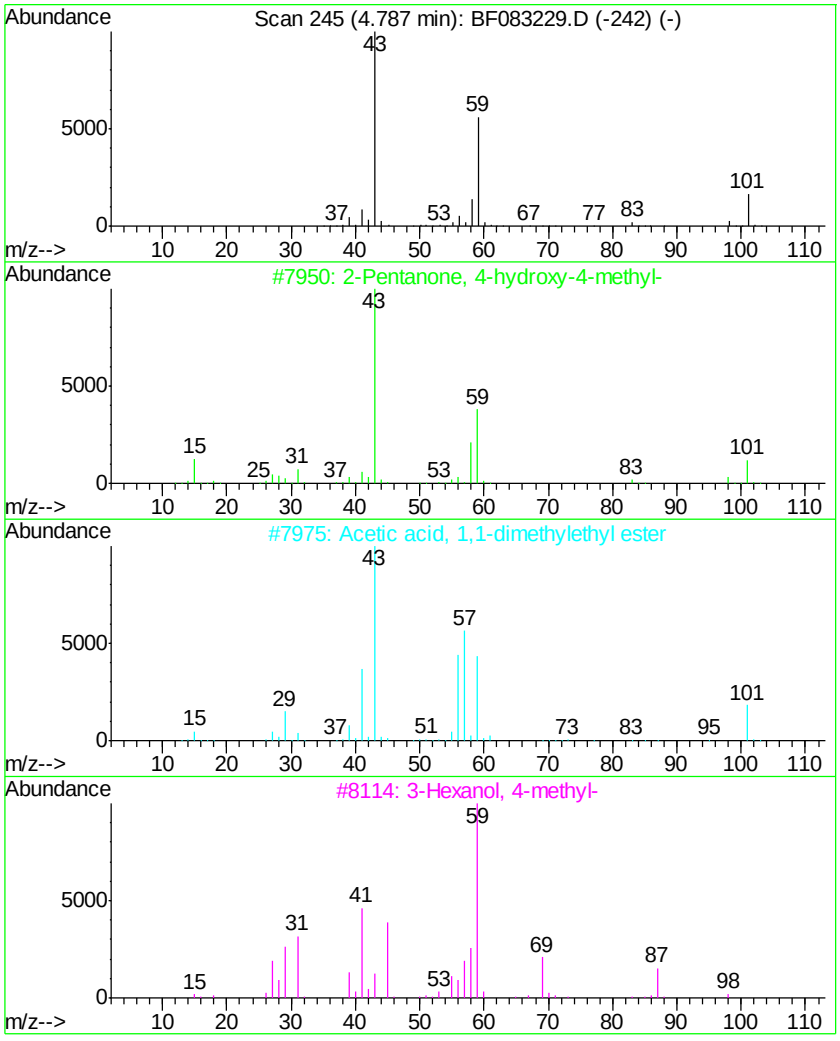
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

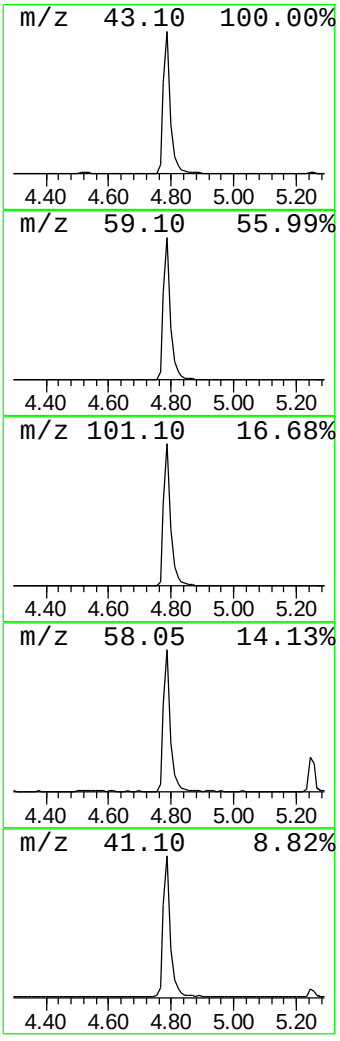
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	37.17 ng	2706580	1,4-Dichlorobenzene-d4	6.64

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	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

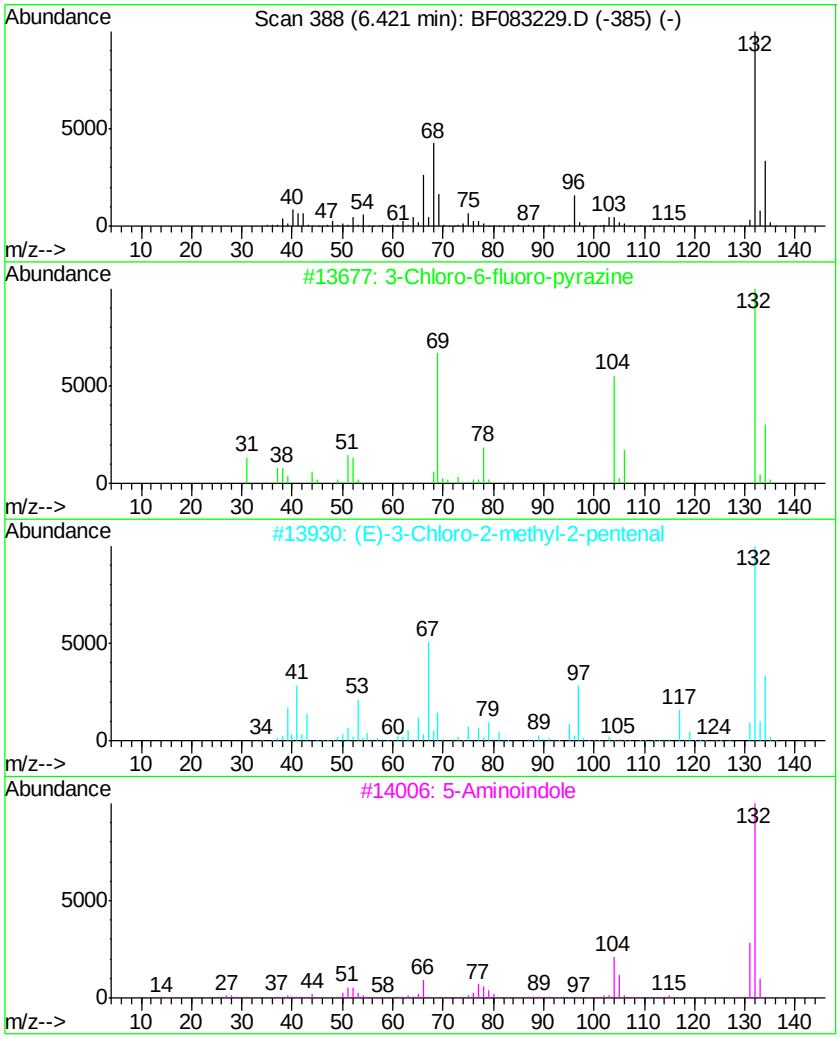
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

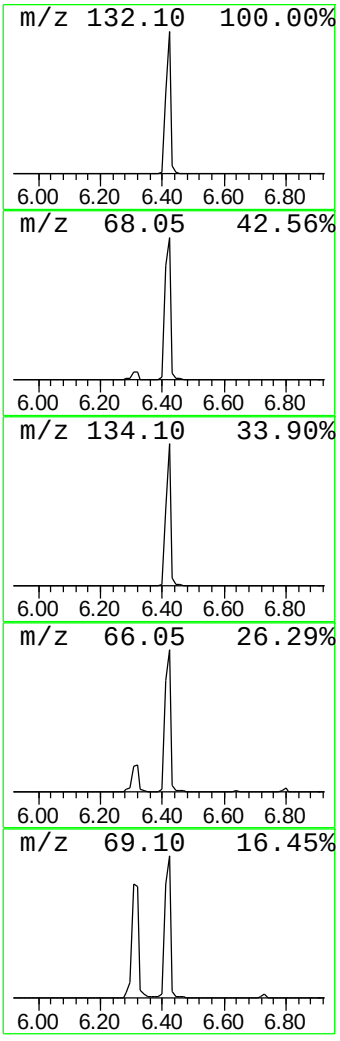
****

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	75.04 ng	5464780	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
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Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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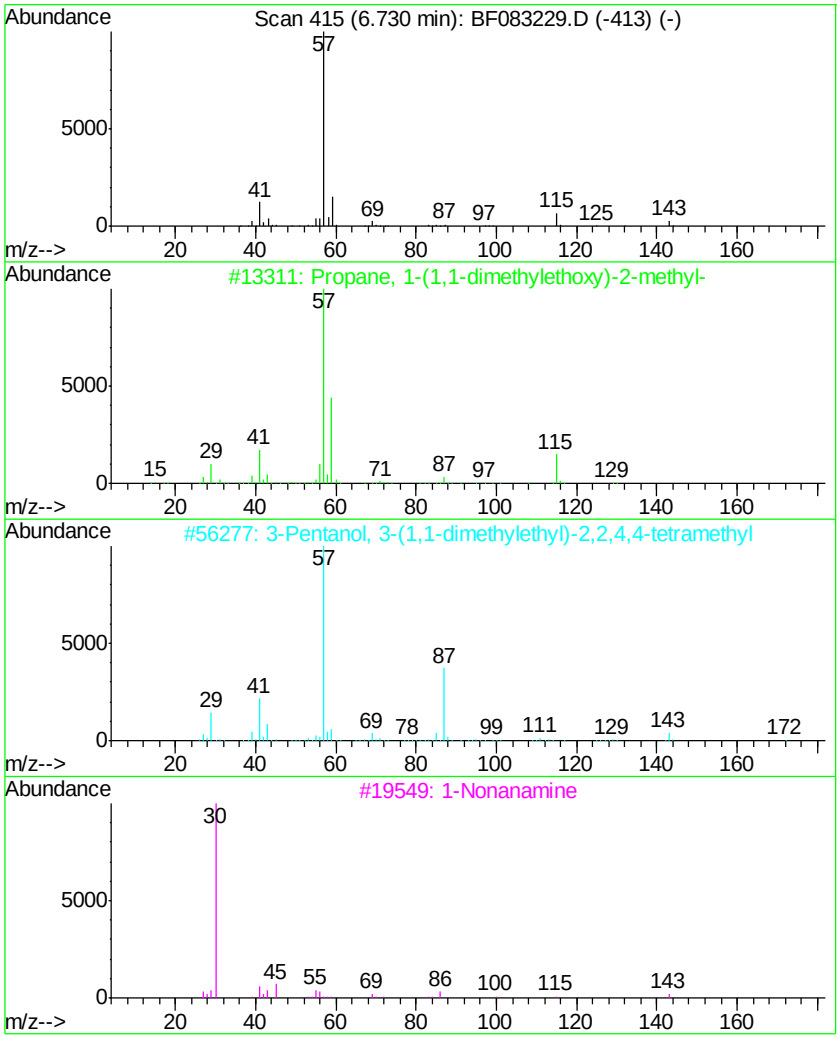
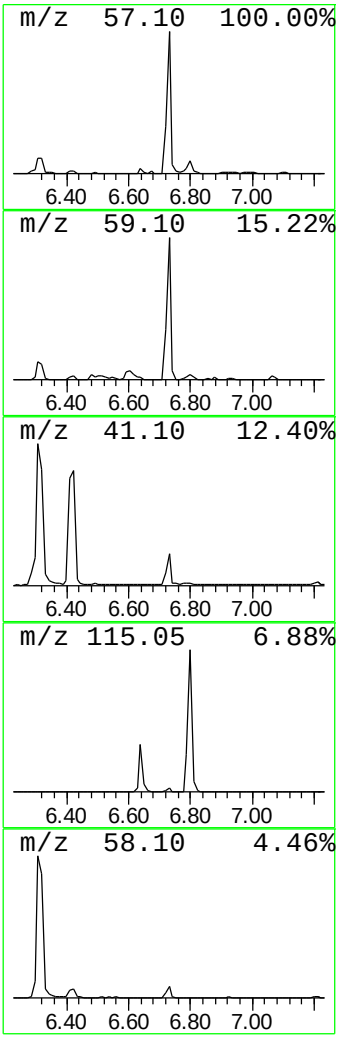
Peak Number 3 unknown6.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	4.03 ng	293389	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(1,1-dimethylethoxy)-...	130	C8H18O	033021-02-2	23
2	3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	12
3	1-Nonanamine	143	C9H21N	000112-20-9	9
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	9
5	Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

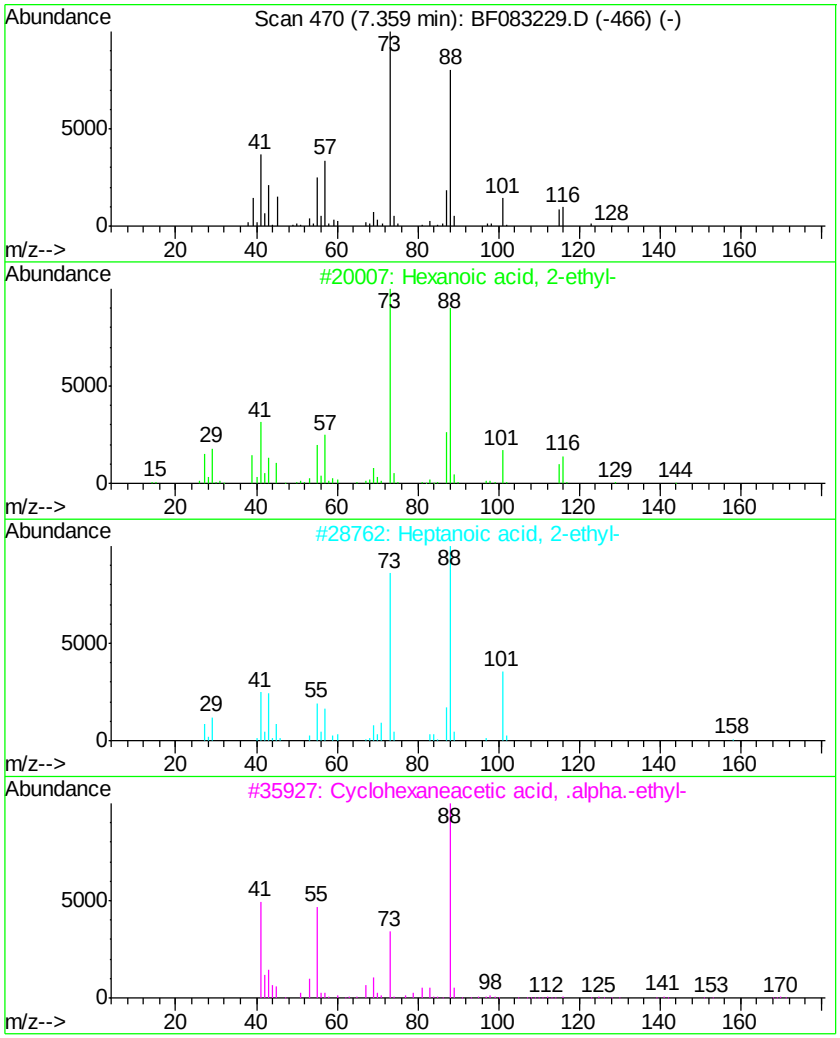
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

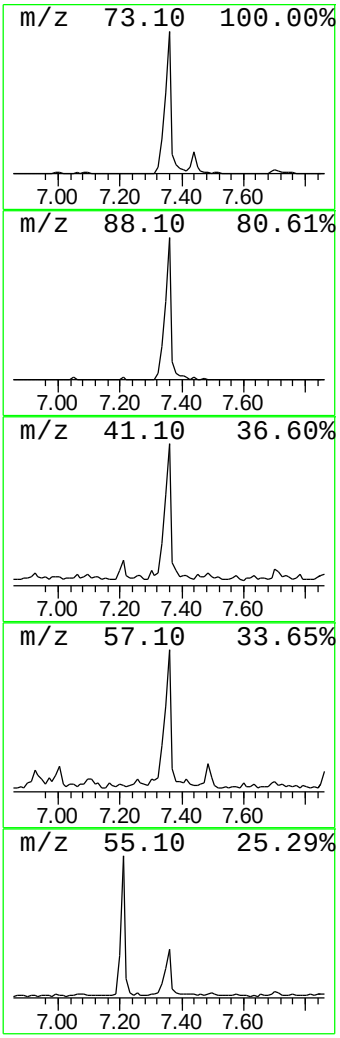
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	2.47 ng	233292	Naphthalene-d8	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	40
4	1,4-Dioxane	88	C4H8O2	000123-91-1	40
5	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	39





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

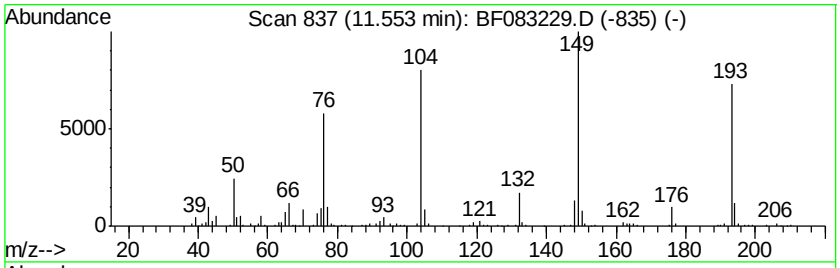
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

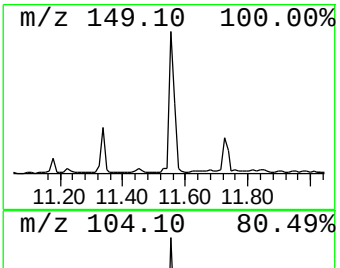
****

Peak Number 6 unknown11.55 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.38 ng	314100	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	38
2	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	38
3	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	35
4	Spiro[isobenzofuran-1(3H),2'-oxi...	220	C11H8O5	1000221-40-6	32
5	Phthalic anhydride	148	C8H4O3	000085-44-9	27





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Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

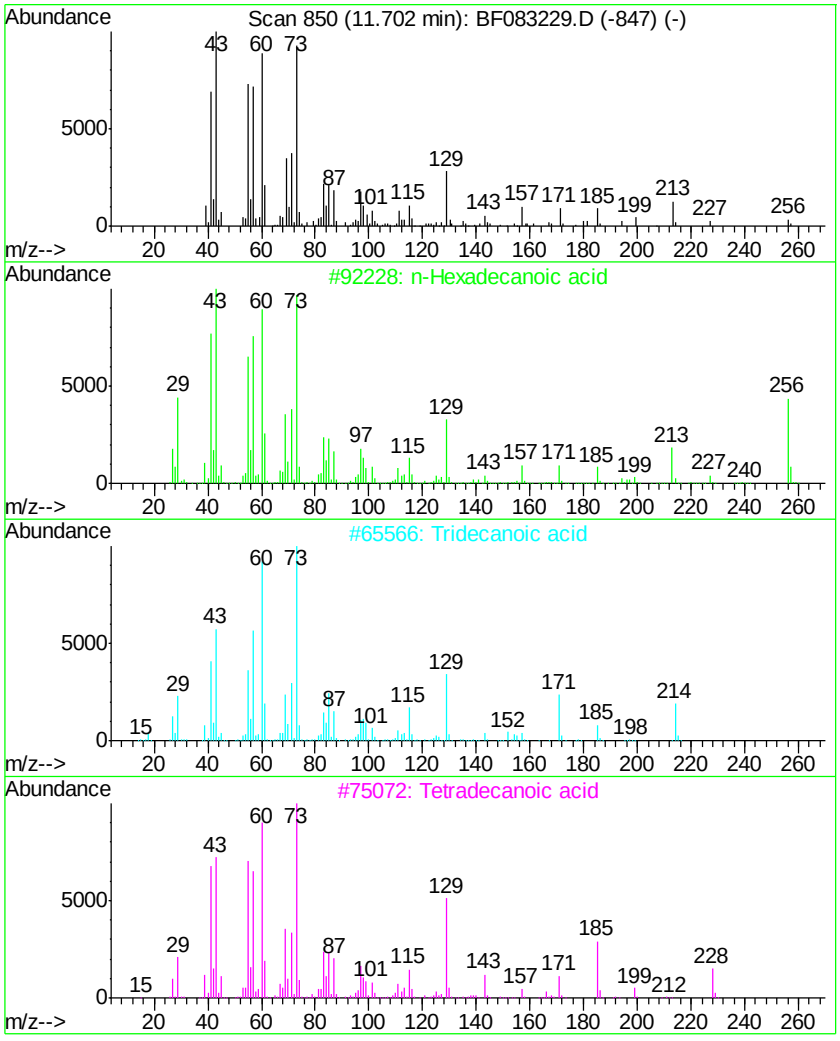
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

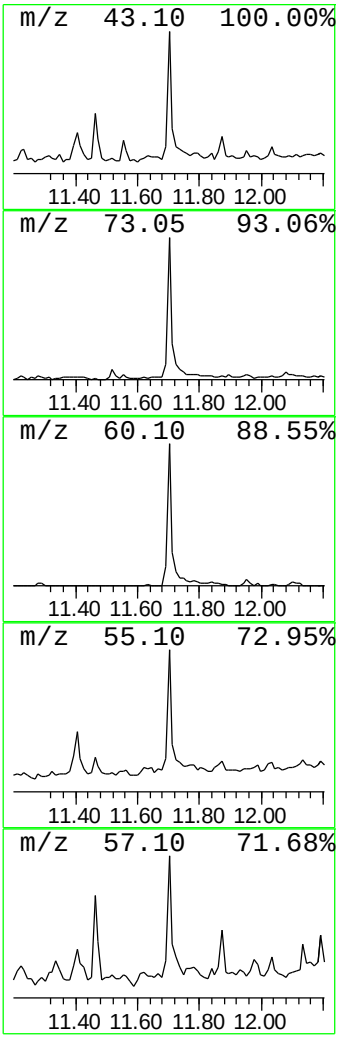
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	3.13 ng	412907	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

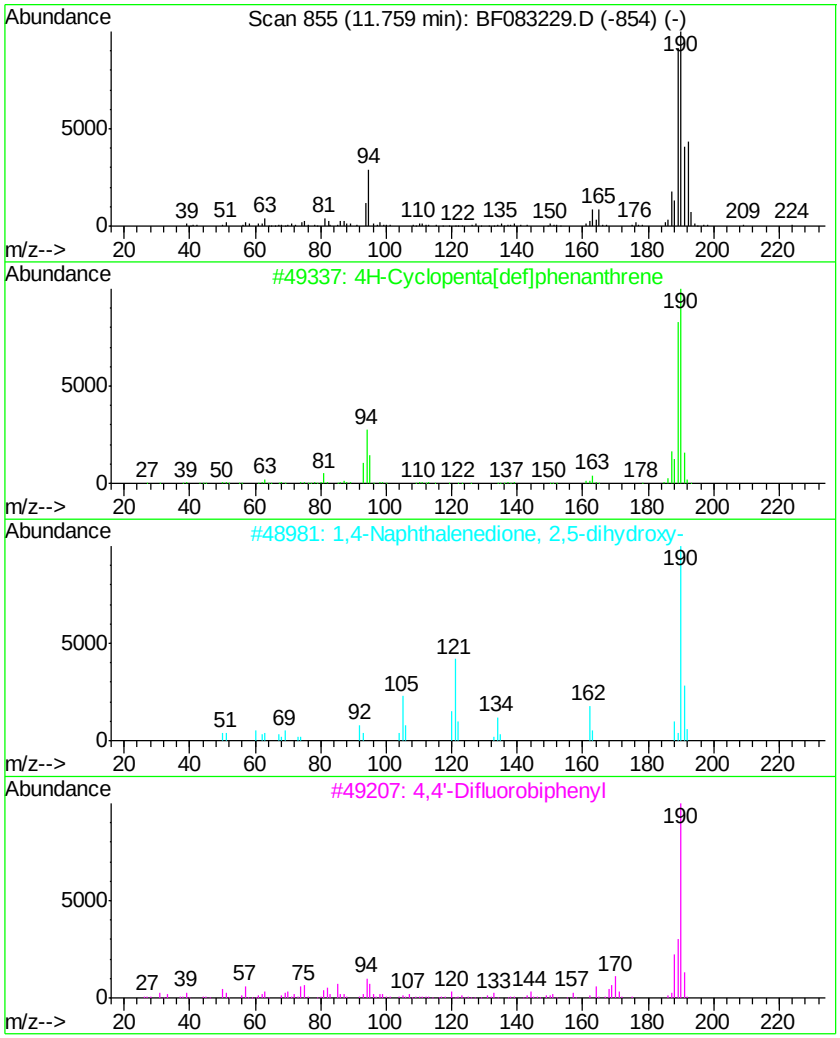
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

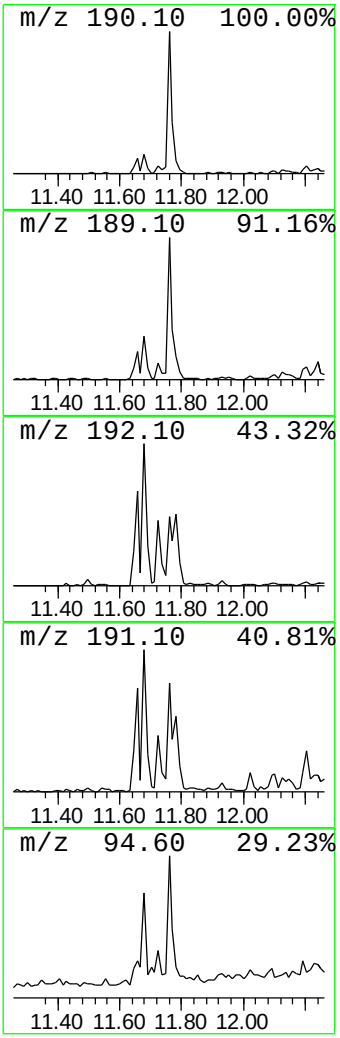
****

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.73 ng	360620	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
3	4,4'-Difluorobiphenyl	190	C12H8F2	000398-23-2	25
4	4-Isothiazolecarbonitrile, 5-chl...	190	C5H3ClN2S2	054798-93-5	16
5	2-Naphthaldehyde, 1,2,3,4-tetrah...	190	C12H14O2	002472-02-8	11





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Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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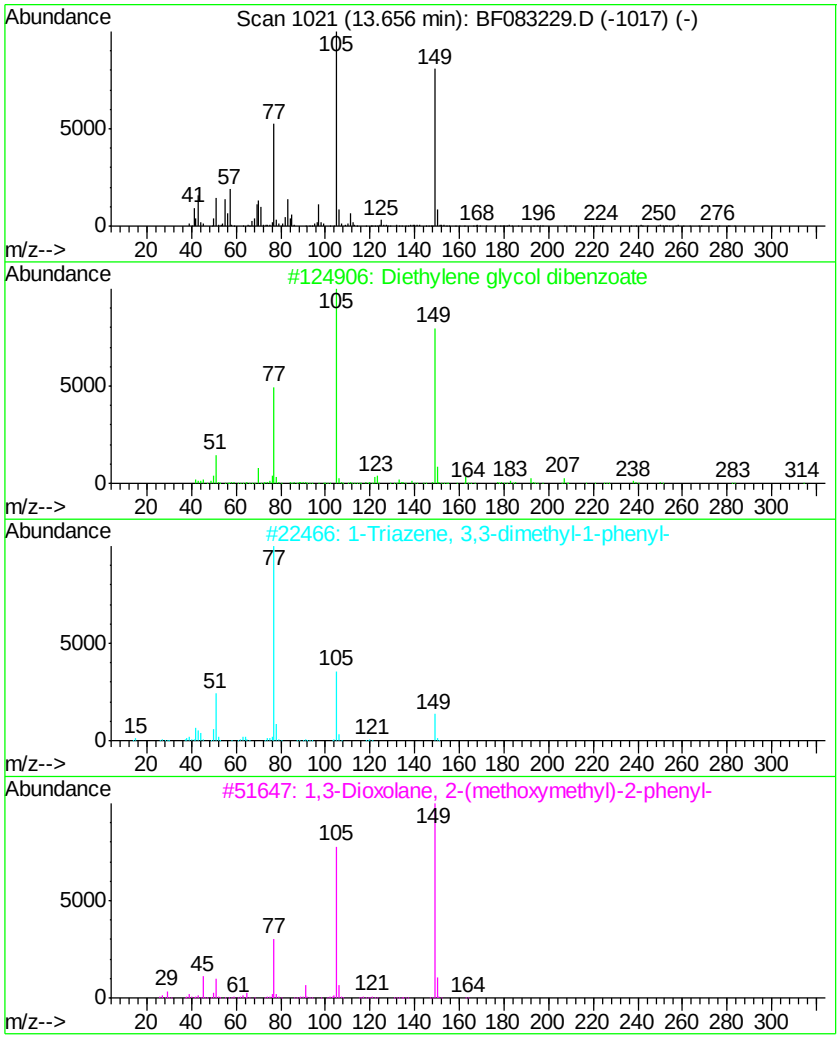
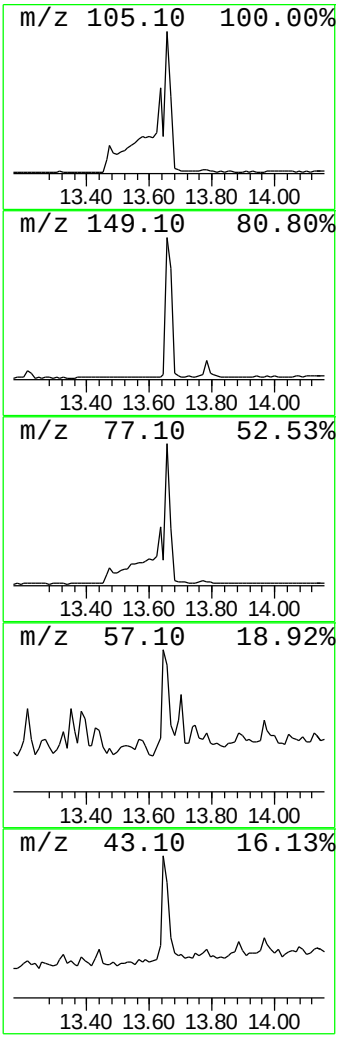
Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	7.13 ng	1037400	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2	1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	50
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
4	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	43
5	N-Benzyl-2-aminocinnamate, methy...	267	C17H17NO2	1000079-39-0	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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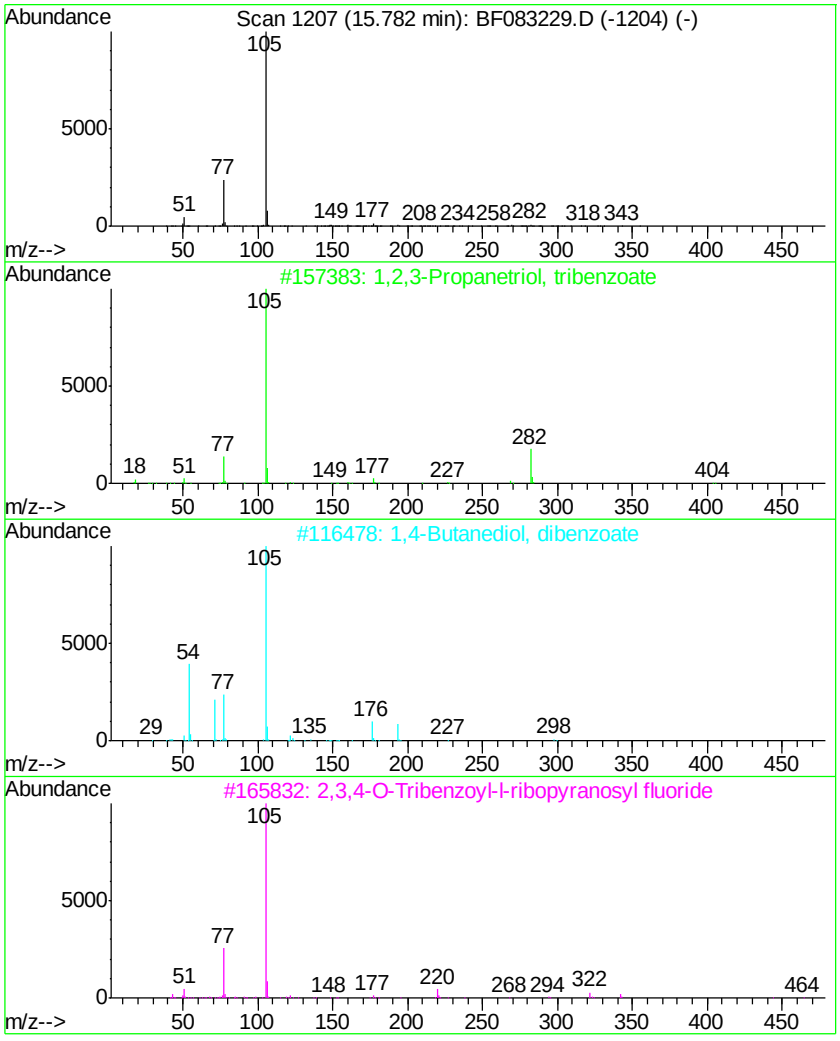
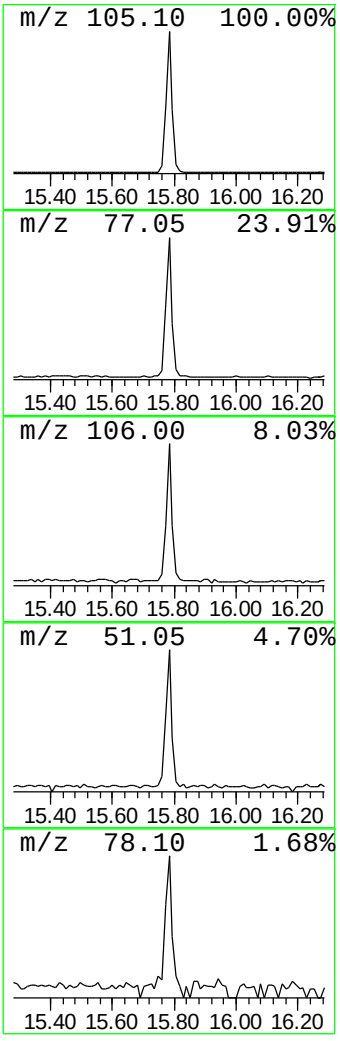
Peak Number 13 1,2,3-Propanetriol, tribenz... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	10.95 ng	624960	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Propanetriol, tribenzoate	404	C24H20O6	000614-33-5	72
2	1,4-Butanediol, dibenzoate	298	C18H18O4	019224-27-2	72
3	2,3,4-O-Tribenzoyl-l-ribopyranos...	464	C26H21FO7	1000129-81-2	72
4	1,3-Oxazolidine-4-carboxylic aci...	291	C16H21NO4	1000196-90-4	64
5	Isopropyl phenyl ketone	148	C10H12O	000611-70-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112315\
Data File : BF083229.D
Acq On : 24 Nov 2015 3:29
Operator : UM/IZ
Sample : G4480-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIBERTY SF_002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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...	4.79	37.2	ng	2706580	1	6.64	1456480	20.0
unknown6.42	6.42	75.0	ng	5464780	1	6.64	1456480	20.0
unknown6.73	6.73	4.0	ng	293389	1	6.64	1456480	20.0
Hexanoic acid, 2-...	7.36	2.5	ng	233292	2	7.93	1888340	20.0
unknown11.55	11.55	2.4	ng	314100	4	11.15	2639960	20.0
n-Hexadecanoic acid	11.70	3.1	ng	412907	4	11.15	2639960	20.0
4H-Cyclopenta[def...	11.76	2.7	ng	360620	4	11.15	2639960	20.0
Diethylene glycol...	13.66	7.1	ng	1037400	5	13.78	2907970	20.0
1,2,3-Propanetrio...	15.78	10.9	ng	624960	6	15.14	1141760	20.0