LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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	4.776	241	244	252	rBV	548652	949034	18.32%	2.074%
2	5.233	282	284	295	rBV	1715655	1977310	38.17%	4.320%
3	5.576	312	314	318	rBV	69087	130966	2.53%	0.286%
4	5.633	318	319	328	rVB	33265	61169	1.18%	0.134%
5	6.296	376	377	385	rBV	985819	1471247	28.40%	3.215%
6	6.410	385	387	390	rBV	3855548	3523832	68.02%	7.699%
7	6.639	405	407	409	rBV	1496500	1430117	27.60%	3.125%
8	6.719	411	414	418	rVB	35465	61011	1.18%	0.133%
9	6.799	418	421	423	rBV	2458216	3089346	59.63%	6.750%
10	7.210	454	457	459	rBV	3047846	3161100	61.02%	6.907%
11	7.370	466	471	473	rVB	153204	292585	5.65%	0.639%
12	7.496	480	482	486	rBV2	84412	164568	3.18%	0.360%
13	7.850	510	513	517	rBV3	41692	107489	2.07%	0.235%
14	7.930	517	520	522	rVV	1641231	1864571	35.99%	4.074%
15	7.965	522	523	528	rVB3	69097	94705	1.83%	0.207%
16	8.090	529	534	537	rBV4	32190	96022	1.85%	0.210%
17	8.308	550	553	556	rVB3	36196	70374	1.36%	0.154%
18	8.376	556	559	561	rBV4	58355	110469	2.13%	0.241%
19	8.525	570	572	575	rBV3	56266	66981	1.29%	0.146%
20	8.673	582	585	587	rBV	99113	160562	3.10%	0.351%
21	8.719	587	589	591	rVB	68264	72643	1.40%	0.159%
22	8.890	601	604	606	rBV2	41451	54951	1.06%	0.120%
23	8.936	606	608	611	rBV2	73399	94312	1.82%	0.206%
24	9.005	611	614	617	rBV	4605940	4656483	89.88%	10.174%
25	9.142	623	626	628	rBV2	37538	56221	1.09%	0.123%
26	9.405	647	649	652	rBV	146967	168524	3.25%	0.368%
27	9.622	665	668	670	rBV2	83911	131225	2.53%	0.287%
28	9.679	670	673	675	rVV	1569137	1977838	38.18%	4.321%
29	9.759	677	680	681	rBV3	33689	69914	1.35%	0.153%
30	9.873	688	690	692	rBV2	61117	99474	1.92%	0.217%
31	10.068	706	707	708	rBV	114826	89918	1.74%	0.196%
32	10.125	711	712	713	rVV	119619	90193	1.74%	0.197%
33	10.205	717	719	721	rVB	100554	127876	2.47%	0.279%
34	10.411	735	737	739	rBV2	58925	95764	1.85%	0.209%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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	10.456	739	741	744	rVV2	1990471	2837463	54.77%	6.200%
36	10.571	748	751	752	rBV2	117420	168873	3.26%	0.369%
37	10.594	752	753	757	rVB	324028	358223	6.91%	0.783%
38	10.914	779	781	785	rBV	188614	267987	5.17%	0.586%
39	11.062	790	794	796	rBV3	92375	144778	2.79%	0.316%
40	11.154	799	802	804	rBV	1885984	1842370	35.56%	4.025%
41	11.462	827	829	831	rBV2	54066	53470	1.03%	0.117%
42	11.702	849	850	853	rBV	341078	446557	8.62%	0.976%
43	12.217	893	895	899	rVB	259405	283073	5.46%	0.618%
44	12.491	917	919	921	rBV	267192	369356	7.13%	0.807%
45	12.731	938	940	943	rVV	3109829	3879935	74.89%	8.477%
46	12.799	943	946	948	rVB	57777	81062	1.56%	0.177%
47	13.211	980	982	986	rVB2	83733	130706	2.52%	0.286%
48	13.325	989	992	994	rBV	4546721	5180659	100.00%	11.319%
49	13.645	1018	1020	1024	rVB	113054	134394	2.59%	0.294%
50	13.771	1029	1031	1034	rBV	1583081	1627775	31.42%	3.557%
51	13.897	1039	1042	1046	rVB	83597	135140	2.61%	0.295%
52	15.131	1148	1150	1153	rBV	837751	1158129	22.35%	2.530%

Sum of corrected areas: 45768744

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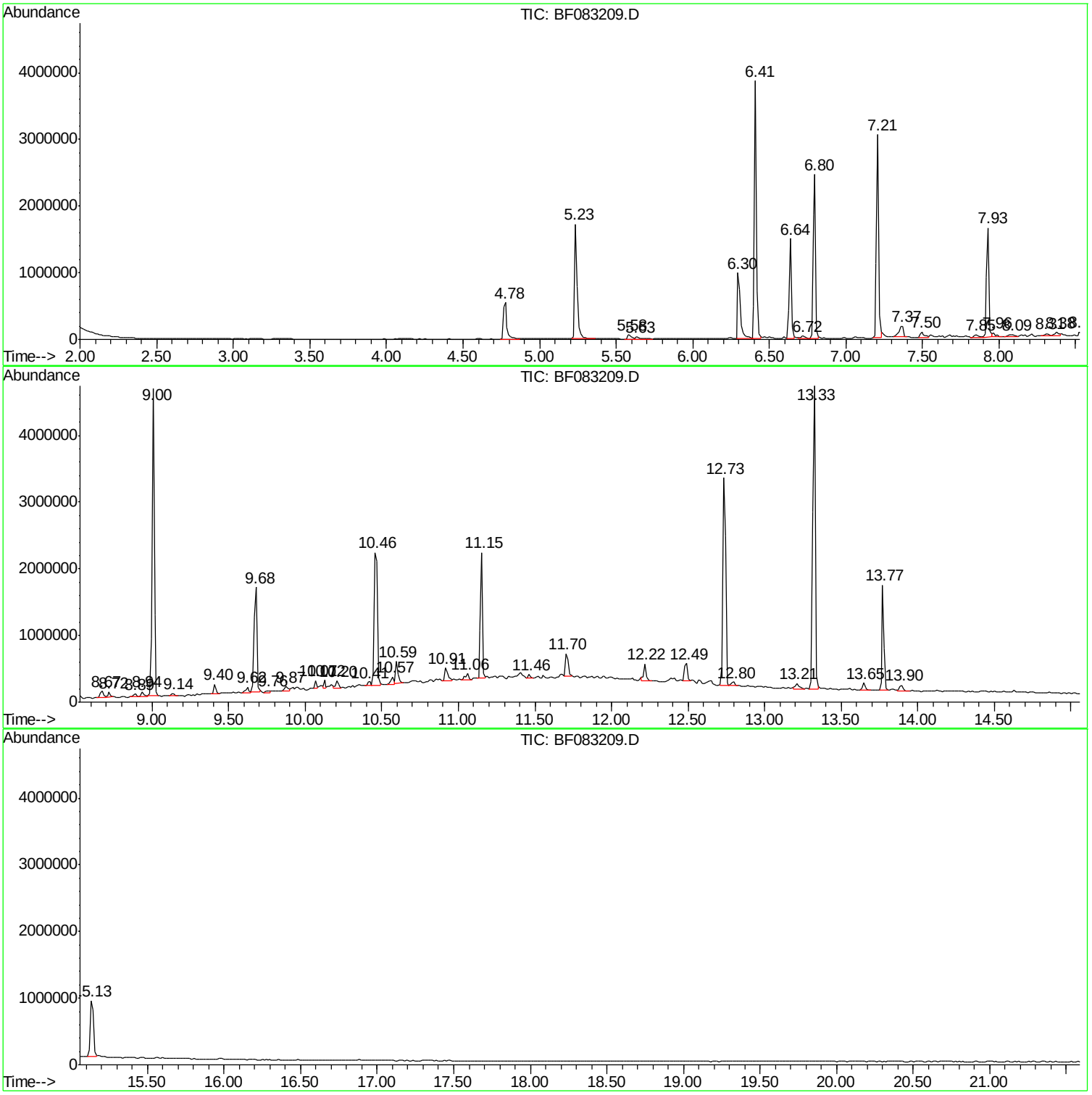
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-12

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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Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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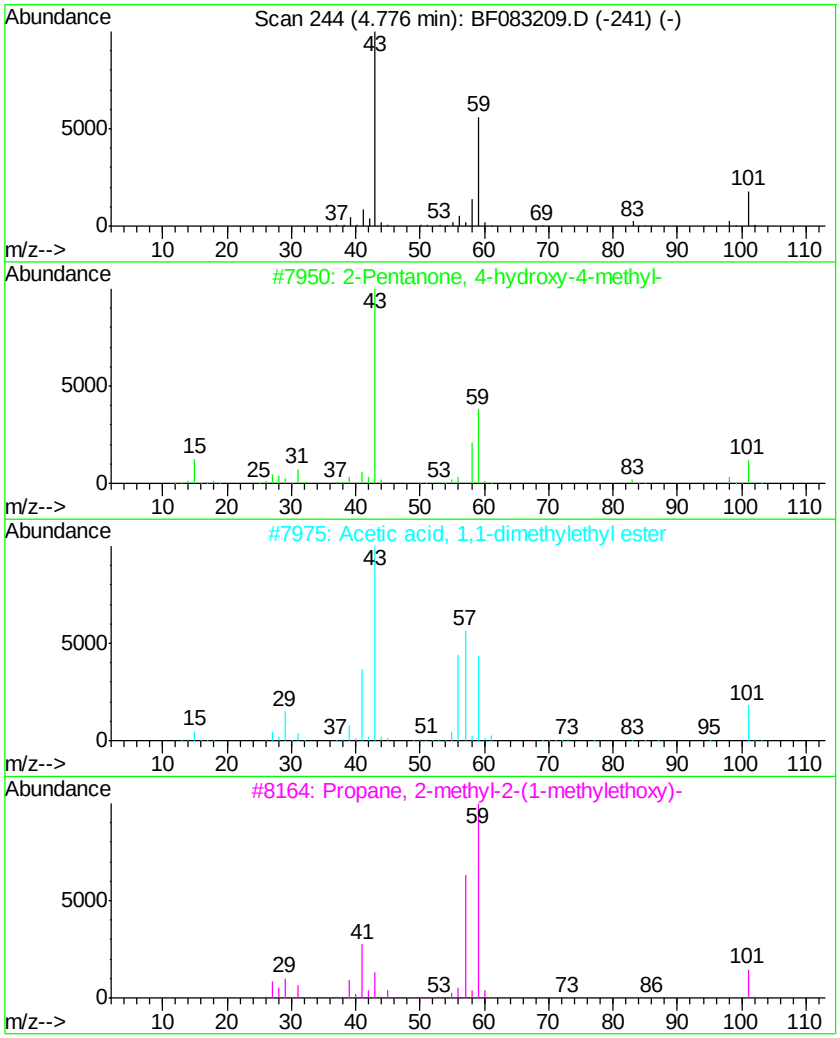
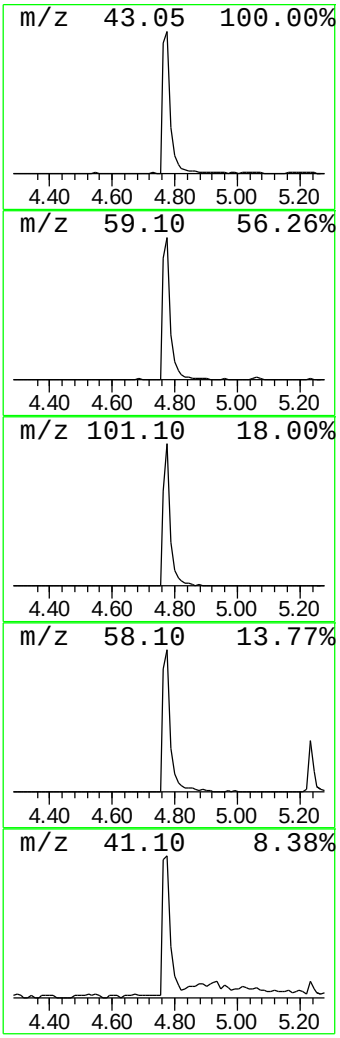
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	13.27 ng	949034	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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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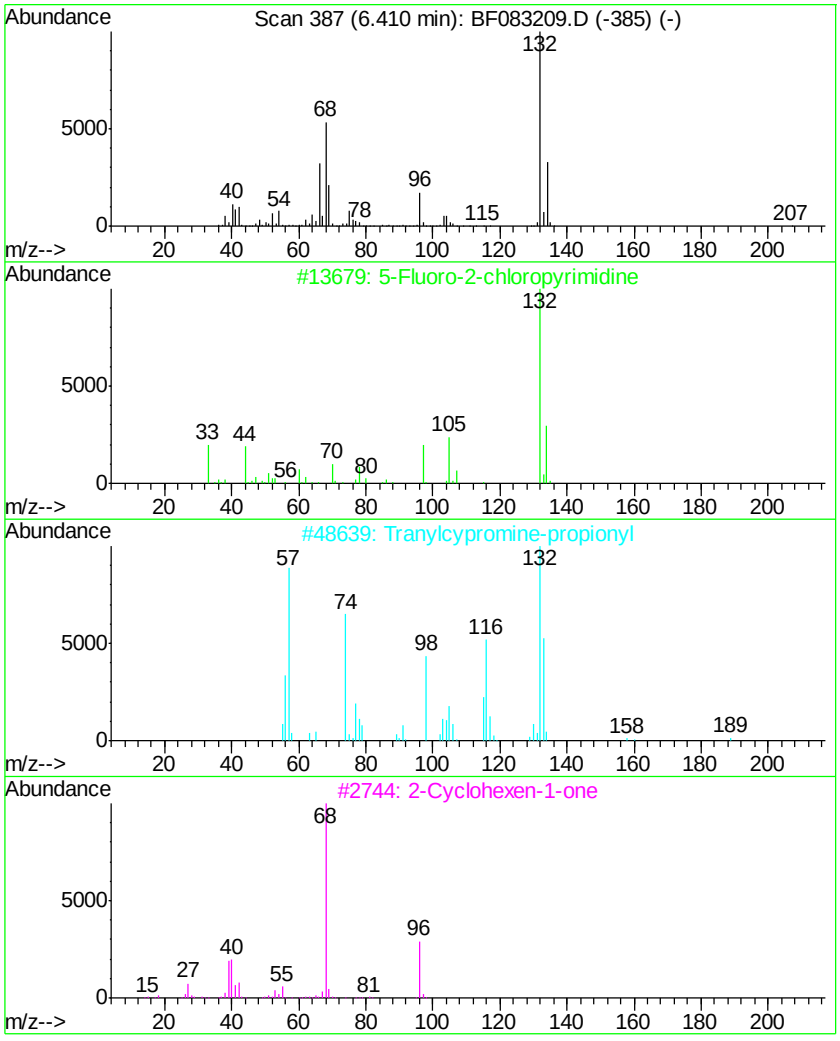
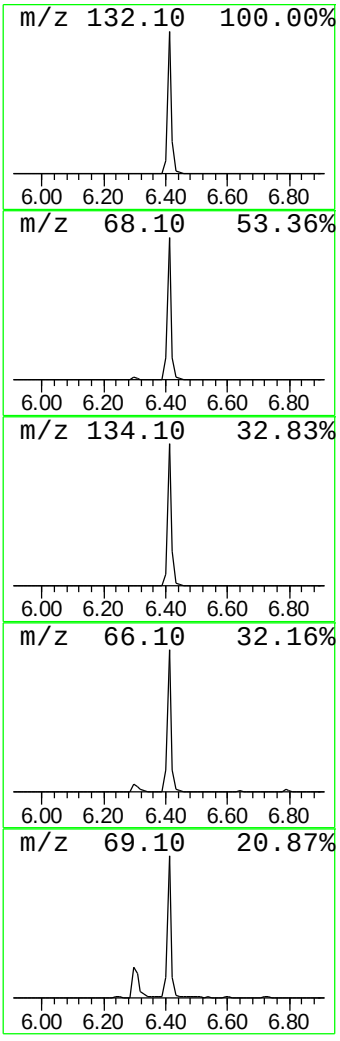
Peak Number 2 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	49.28 ng	3523830	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	Xenon	132	Xe	007440-63-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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

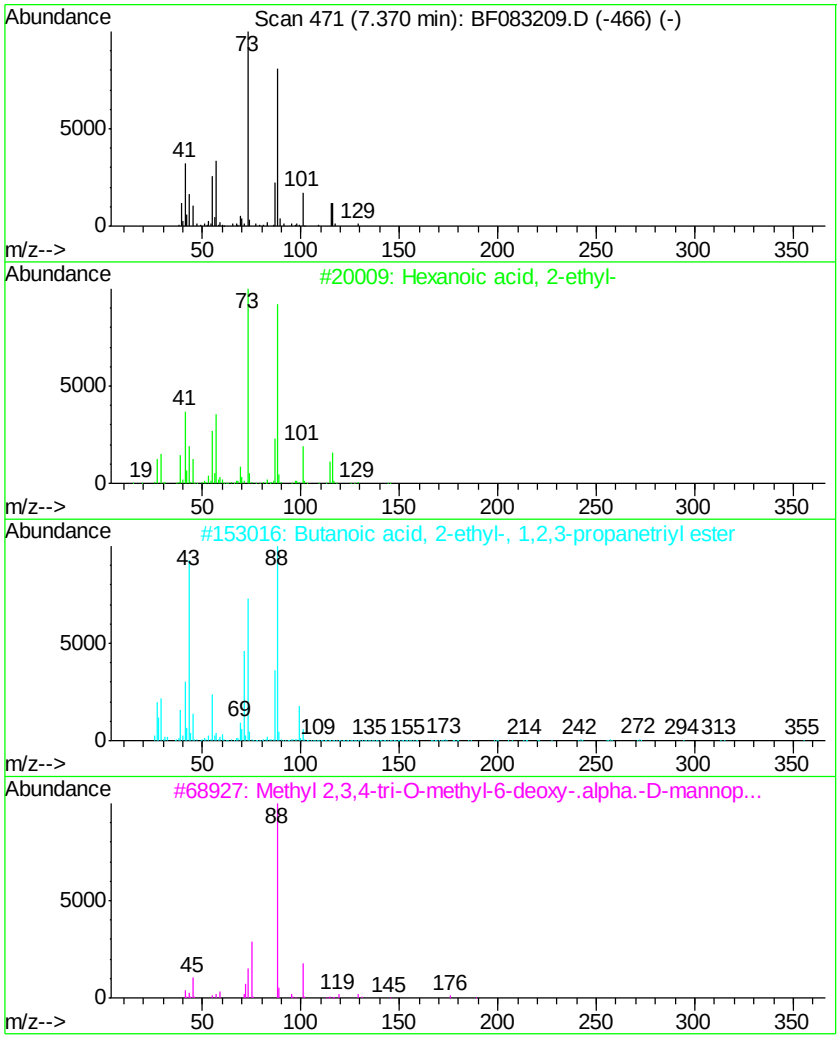
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

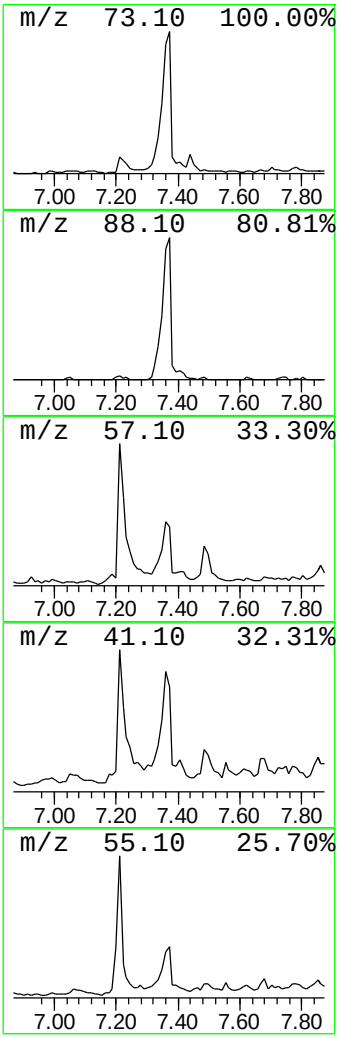
****

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	3.14 ng	292585	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	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
4	1,4-Dioxane	88	C4H8O2	000123-91-1	37
5	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	33





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Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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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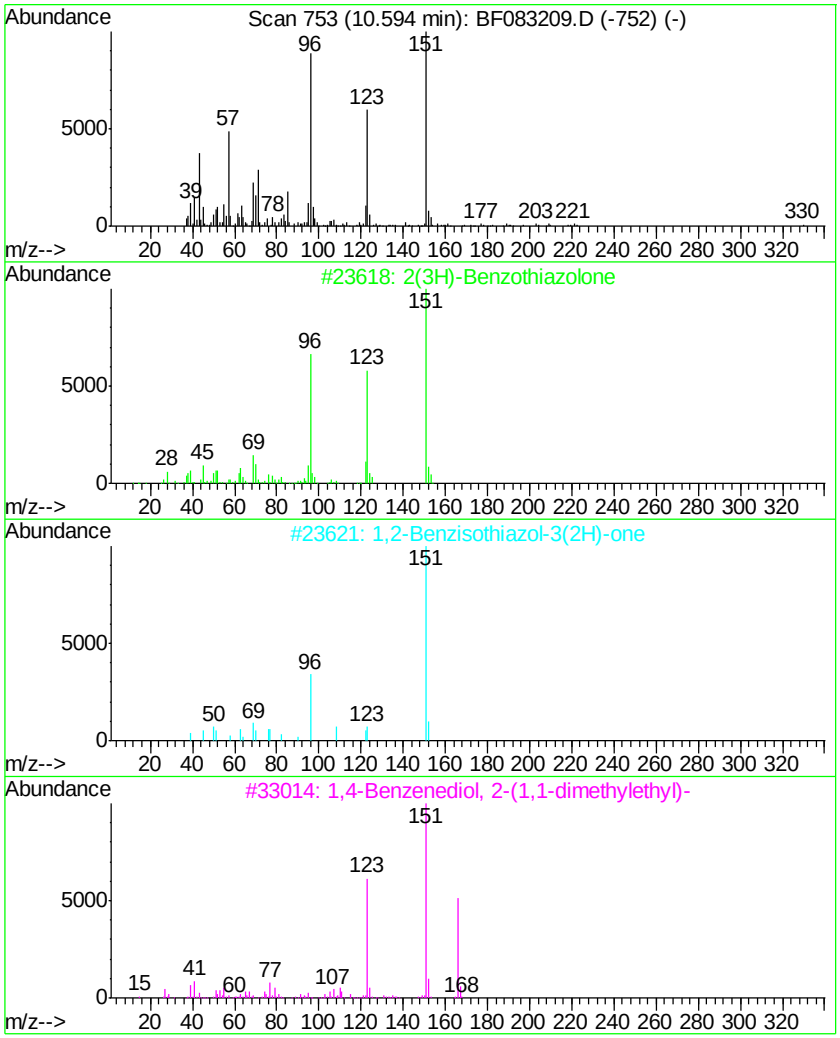
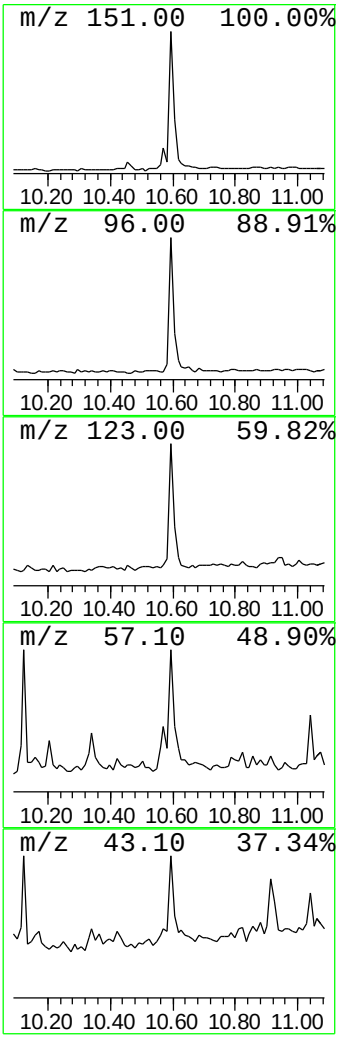
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	3.89 ng	358223	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	52
3	1,4-Benzenediol, 2-(1,1-dimethyl...	166	C10H14O2	001948-33-0	35
4	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	25
5	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	22





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Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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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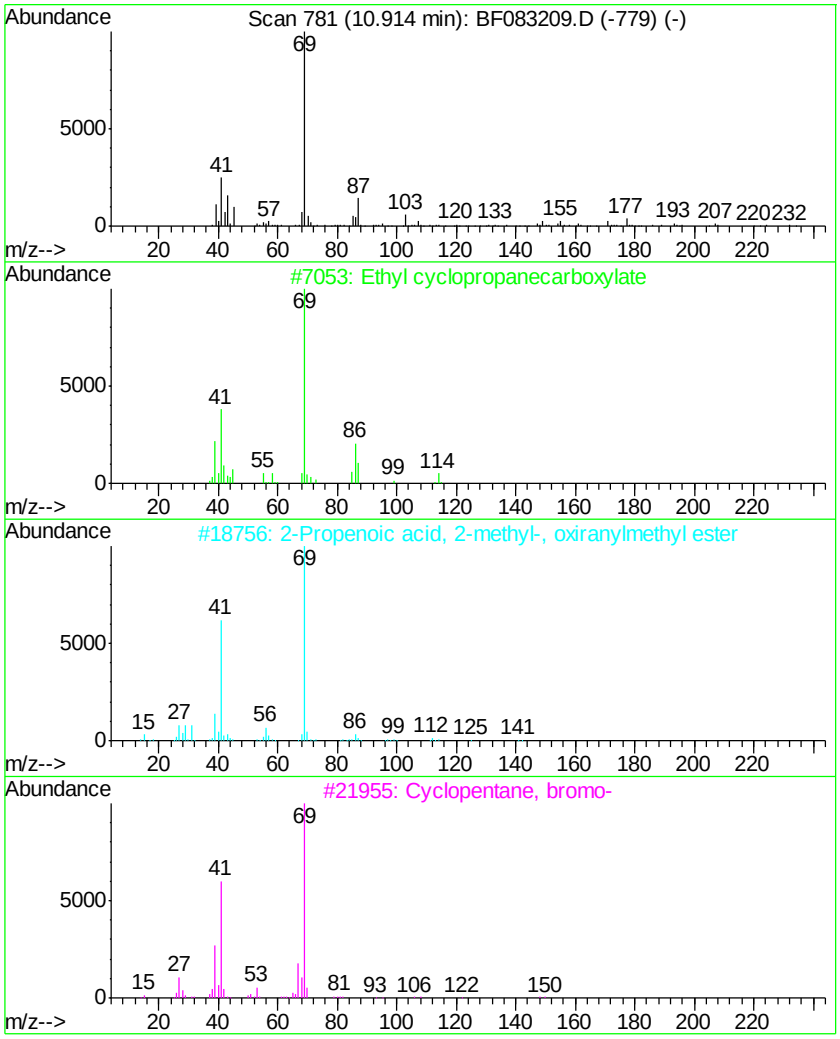
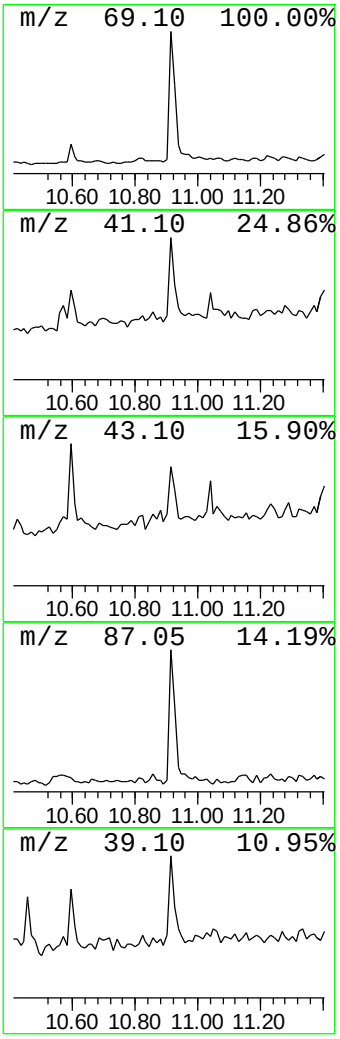
Peak Number 6 unknown10.91 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	2.91 ng	267987	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
2	2-Propenoic acid, 2-methyl-, oxi...	142	C7H10O3	000106-91-2	33
3	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	28
4	3-Butyn-2-ol, 2-methyl-	84	C5H8O	000115-19-5	9
5	2,4-Dinitrophenyl crotonate	252	C10H8N2O6	069817-88-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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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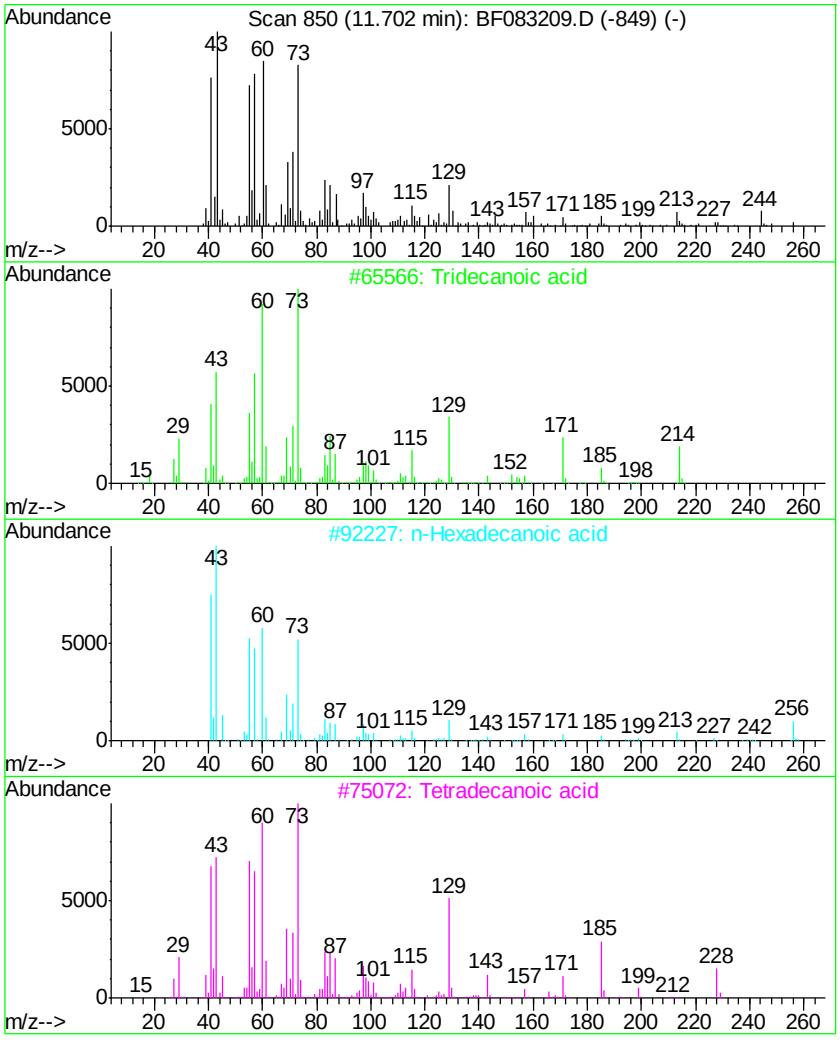
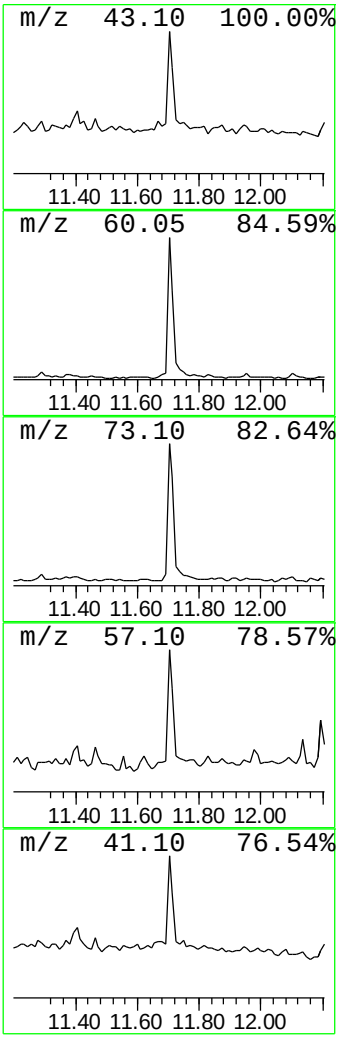
Peak Number 7 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	4.85 ng	446557	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	86





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Misc :
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Instrument : BNA_F
ClientSampleId : MW-12

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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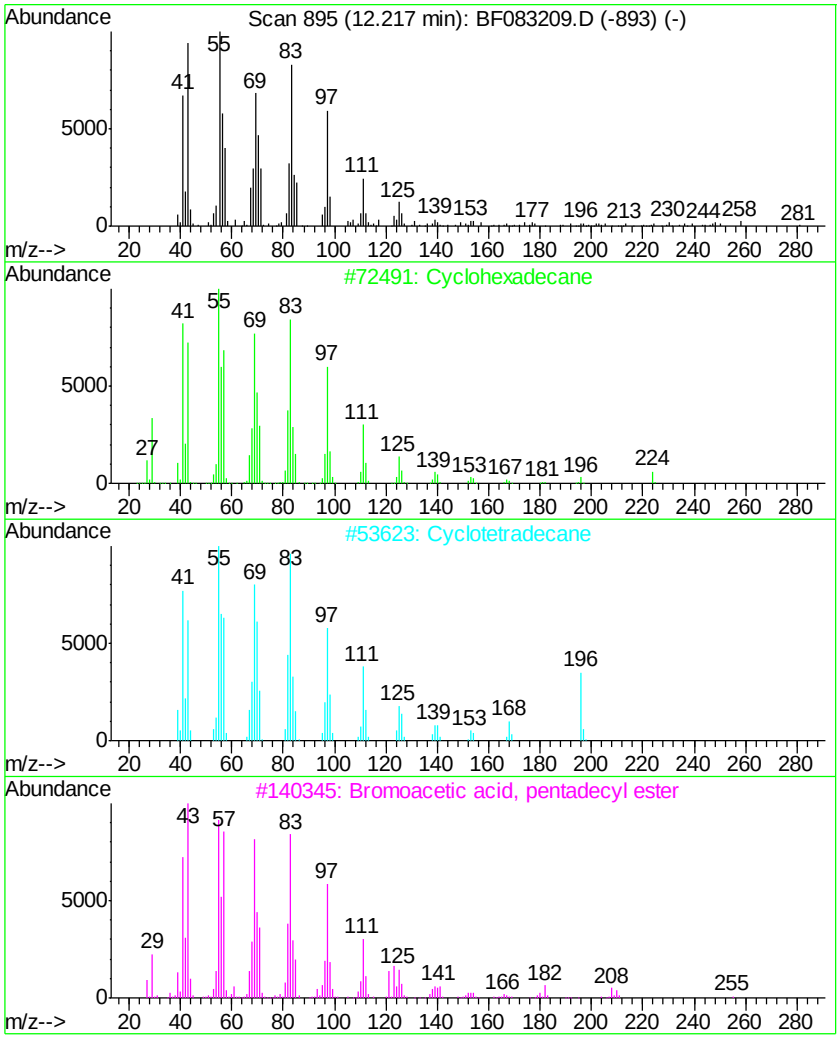
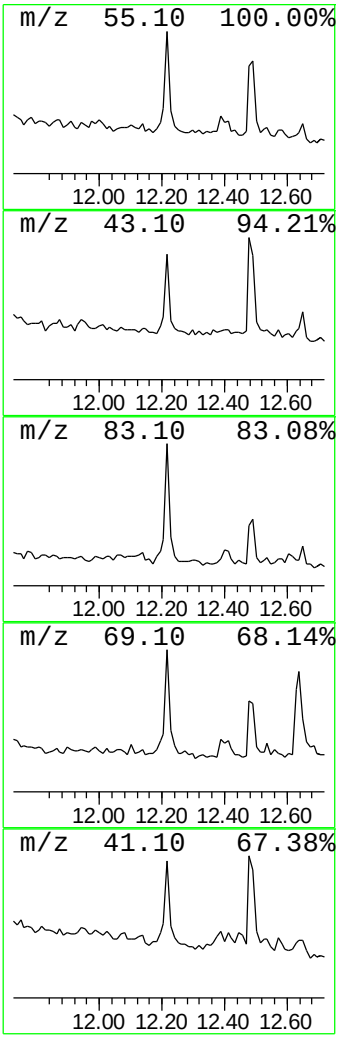
Peak Number 8 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	3.07 ng	283073	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Cyclotetradecane	196	C14H28	000295-17-0	95
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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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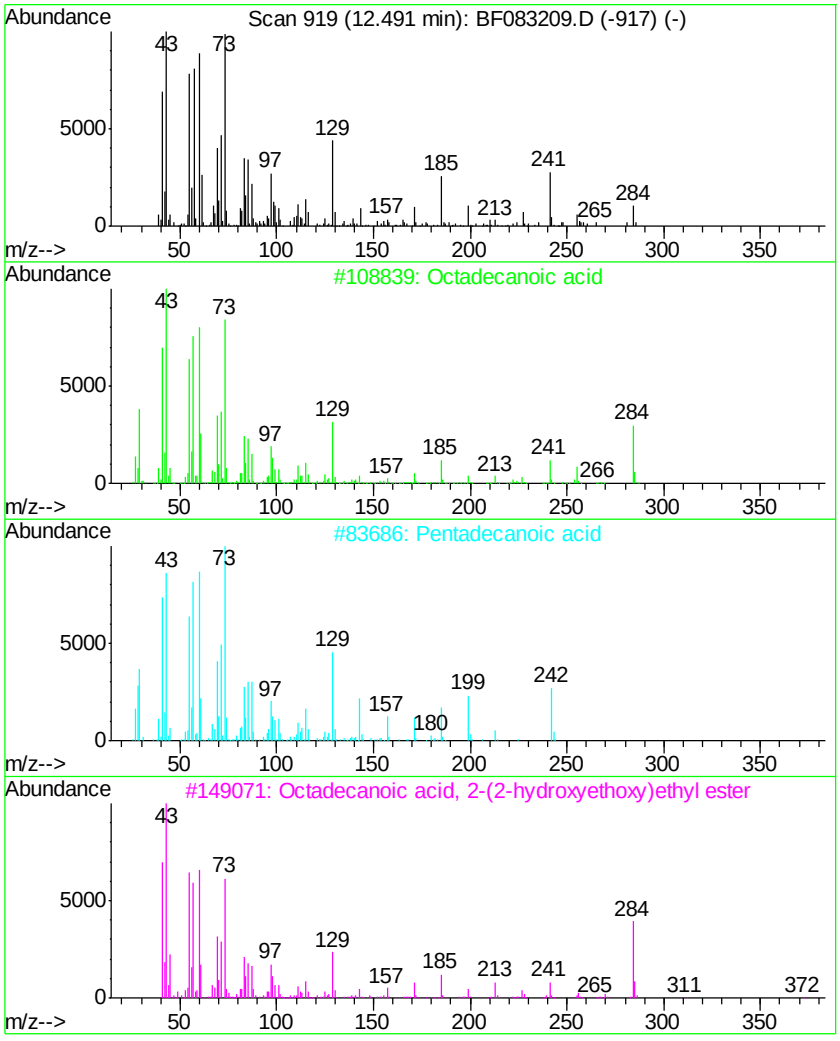
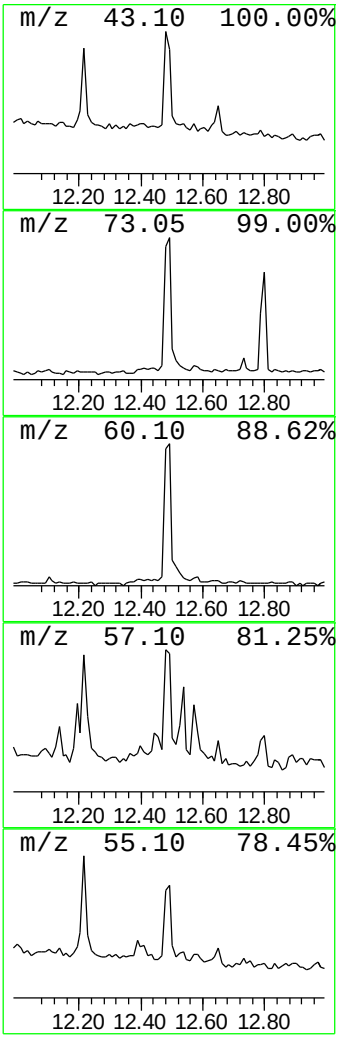
Peak Number 9 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	4.54 ng	369356	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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

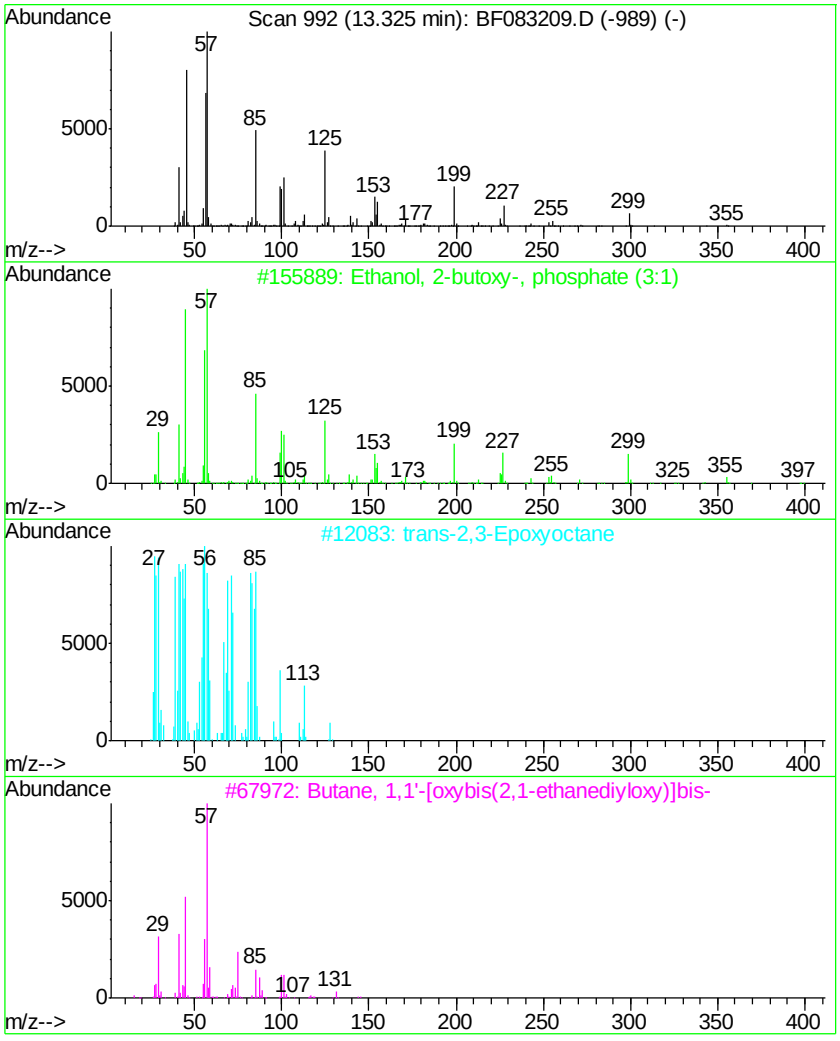
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

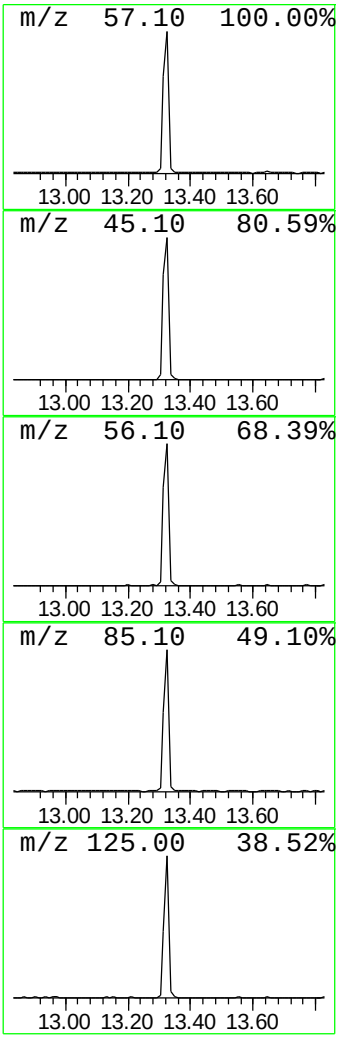
****

Peak Number 10 Ethanol, 2-butoxy-, phospha... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	63.65 ng	5180660	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	72
2	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	47
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	38
4	2,5-Hexanediol	118	C6H14O2	002935-44-6	37
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112315\
Data File : BF083209.D
Acq On : 23 Nov 2015 17:43
Operator : UM/IZ
Sample : G4437-16
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-12

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...	4.78	13.3	ng	949034	1	6.64	1430120	20.0
unknown6.41	6.41	49.3	ng	3523830	1	6.64	1430120	20.0
Hexanoic acid, 2-...	7.37	3.1	ng	292585	2	7.93	1864570	20.0
2(3H)-Benzothiazo...	10.59	3.9	ng	358223	4	11.15	1842370	20.0
unknown10.91	10.91	2.9	ng	267987	4	11.15	1842370	20.0
Tridecanoic acid	11.70	4.8	ng	446557	4	11.15	1842370	20.0
Cyclohexadecane	12.22	3.1	ng	283073	4	11.15	1842370	20.0
Octadecanoic acid	12.49	4.5	ng	369356	5	13.77	1627780	20.0
Ethanol, 2-butoxy...	13.33	63.6	ng	5180660	5	13.77	1627780	20.0