LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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-BF092815.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	4.549	209	211	214	rVB	33605	43223	1.43%	0.207%
2	4.823	233	235	239	rBV	31565	47395	1.57%	0.227%
3	5.040	252	254	258	rBV	275383	330874	10.96%	1.586%
4	5.109	258	260	264	rVV	24942	35481	1.18%	0.170%
5	5.177	264	266	269	rVB2	45944	54858	1.82%	0.263%
6	5.463	288	291	293	rBV	1003000	997986	33.07%	4.784%
7	5.566	296	300	303	rVB2	22957	44377	1.47%	0.213%
8	5.646	303	307	310	rBV4	21789	53515	1.77%	0.257%
9	5.863	324	326	329	rBV	24544	34911	1.16%	0.167%
10	6.194	352	355	361	rBV2	32212	51635	1.71%	0.248%
11	6.492	379	381	384	rBV	439647	550899	18.25%	2.641%
12	6.549	384	386	391	rVB	56691	81463	2.70%	0.391%
13	6.640	391	394	396	rBV	1864849	2003003	66.37%	9.603%
14	6.869	412	414	416	rBV	436359	460713	15.27%	2.209%
15	6.903	416	417	420	rVB2	59048	75016	2.49%	0.360%
16	7.029	425	428	430	rBV	2045471	2058478	68.21%	9.868%
17	7.212	440	444	447	rVB3	50328	68737	2.28%	0.330%
18	7.440	461	464	467	rBV	1351893	1369435	45.38%	6.565%
19	7.520	469	471	473	rVB	35006	56779	1.88%	0.272%
20	7.646	480	482	485	rVB	69327	68178	2.26%	0.327%
21	7.726	485	489	490	rBV	27245	48782	1.62%	0.234%
22	7.840	498	499	501	rVB	38178	34560	1.15%	0.166%
23	7.897	501	504	506	rBV	134338	163970	5.43%	0.786%
24	8.160	524	527	533	rVV	704125	744813	24.68%	3.571%
25	8.275	535	537	541	rVB2	16124	30348	1.01%	0.145%
26	8.423	547	550	553	rBV3	34605	76934	2.55%	0.369%
27	8.526	557	559	564	rVB2	26353	37061	1.23%	0.178%
28	8.686	571	573	575	rBV2	26535	42532	1.41%	0.204%
29	8.755	577	579	581	rBV	36526	43376	1.44%	0.208%
30	8.972	594	598	599	rBV2	27191	54223	1.80%	0.260%
31	9.006	599	601	603	rVB3	20416	36281	1.20%	0.174%
32	9.200	616	618	619	rBV2	22180	31190	1.03%	0.150%
33	9.235	619	621	624	rBV	2280240	2668885	88.43%	12.795%
34	9.418	635	637	642	rVB4	12446	32931	1.09%	0.158%

LSC Area Percent Report

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Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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-BF092815.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.509	642	645	649	rBV3	19931	52385	1.74%	0.251%
36	9.921	678	681	683	rBV	573117	783424	25.96%	3.756%
37	10.526	732	734	737	rVB	44354	45447	1.51%	0.218%
38	10.641	741	744	747	rBV	53366	94858	3.14%	0.455%
39	10.709	747	750	752	rBV	1703971	1789832	59.31%	8.581%
40	10.812	757	759	764	rVV2	24296	52987	1.76%	0.254%
41	10.915	764	768	770	rVB3	20714	36185	1.20%	0.173%
42	11.258	796	798	804	rVB3	15145	37449	1.24%	0.180%
43	11.406	808	811	813	rBV	695660	750452	24.87%	3.598%
44	11.932	854	857	859	rBV	64574	91148	3.02%	0.437%
45	12.709	923	925	930	rBV2	29513	46919	1.55%	0.225%
46	12.995	947	950	952	rBV	2907544	3017912	100.00%	14.468%
47	13.898	1026	1029	1035	rVB3	15262	33070	1.10%	0.159%
48	14.047	1039	1042	1052	rVB	690843	819706	27.16%	3.930%
49	15.487	1165	1168	1183	rBV	471445	674499	22.35%	3.234%

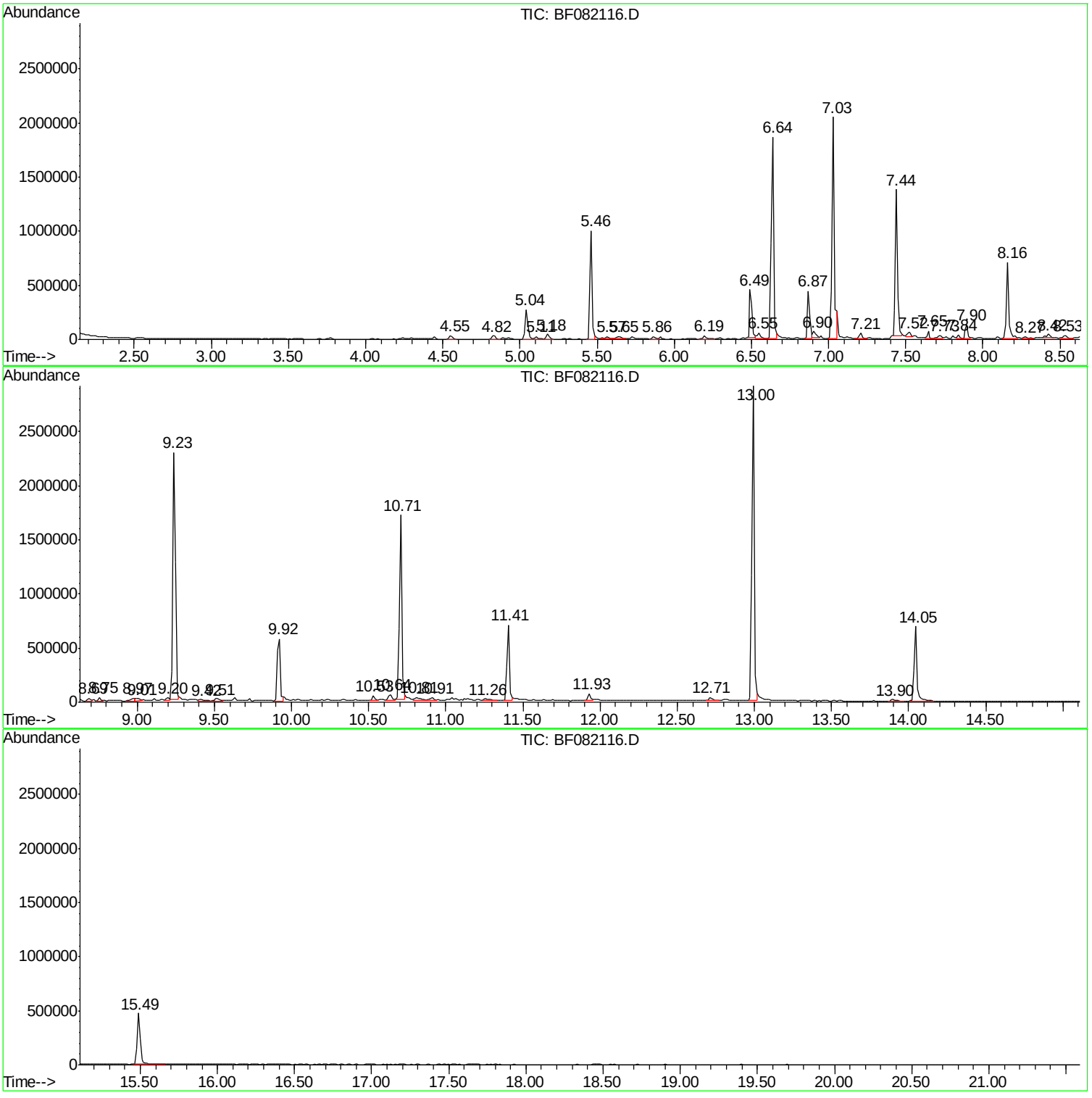
Sum of corrected areas: 20859115

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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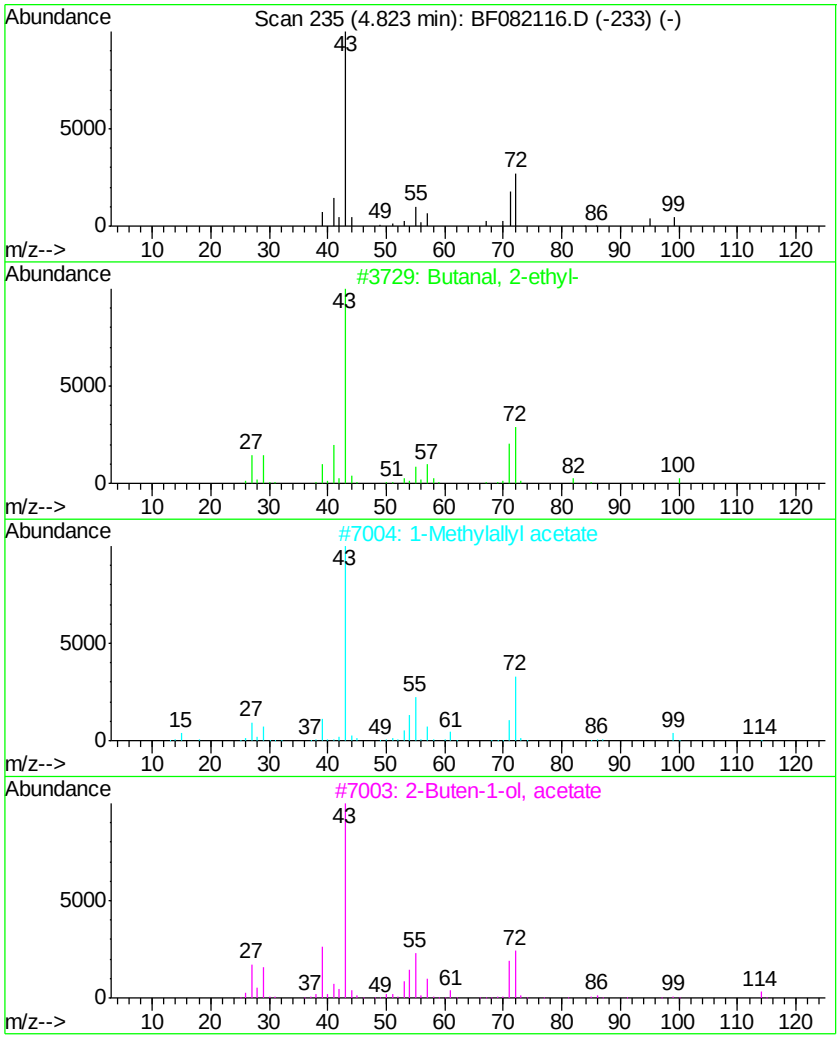
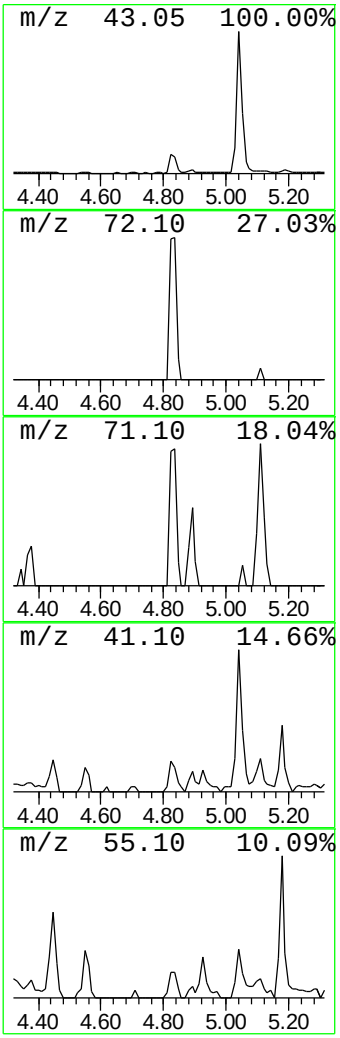
Peak Number 1 Butanal, 2-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	2.06 ng	47395	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	59
2	1-Methylallyl acetate	114	C6H10O2	006737-11-7	38
3	2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	38
4	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	33
5	2-Butanone	72	C4H8O	000078-93-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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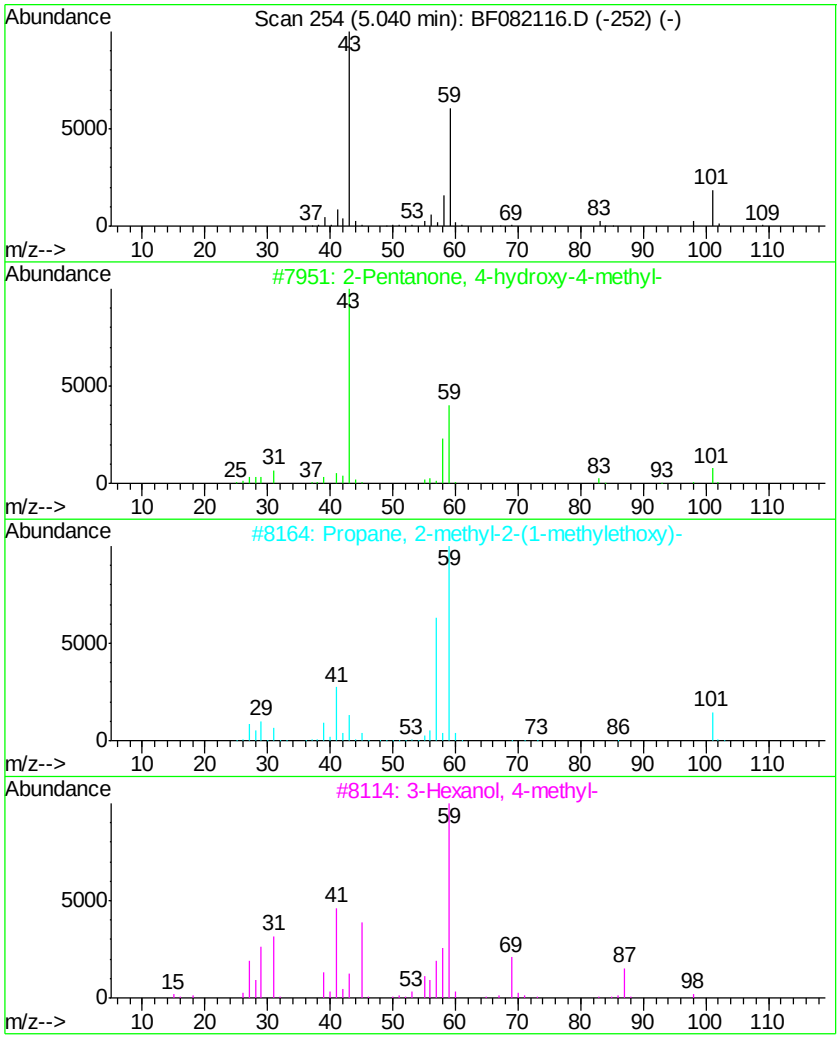
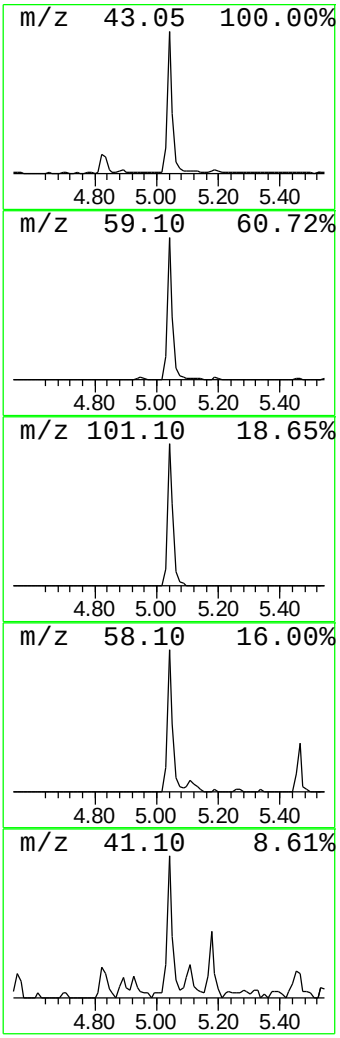
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	14.36 ng	330874	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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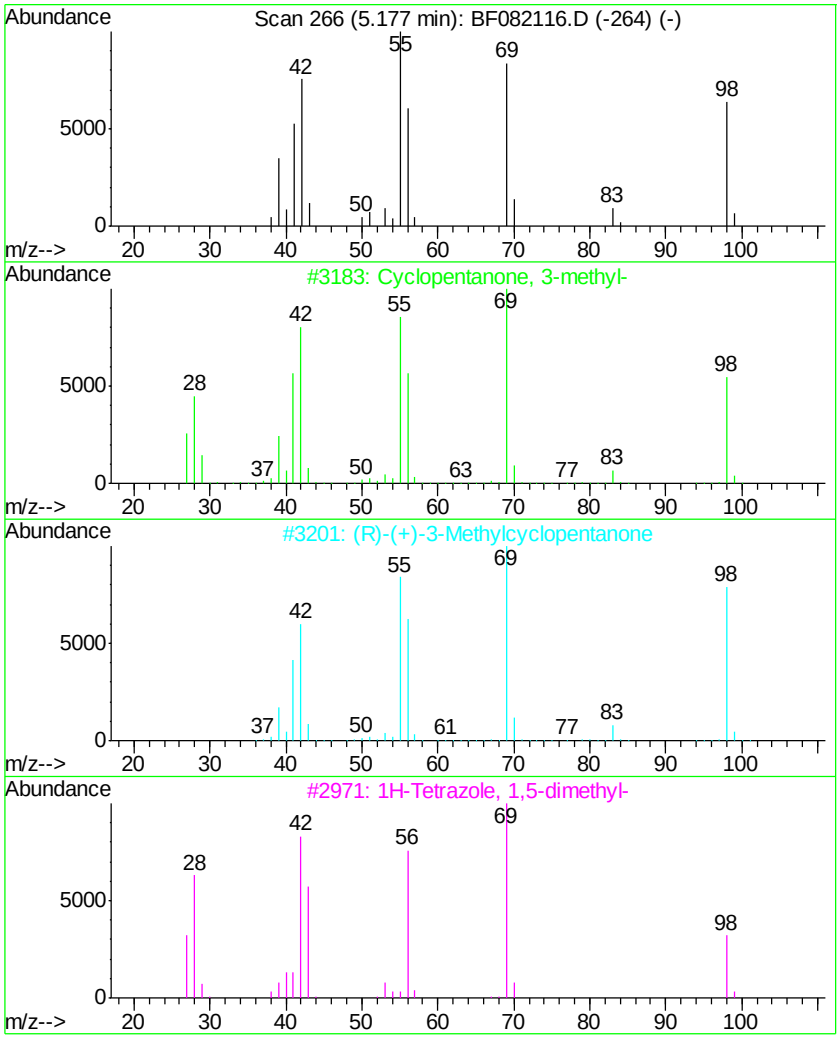
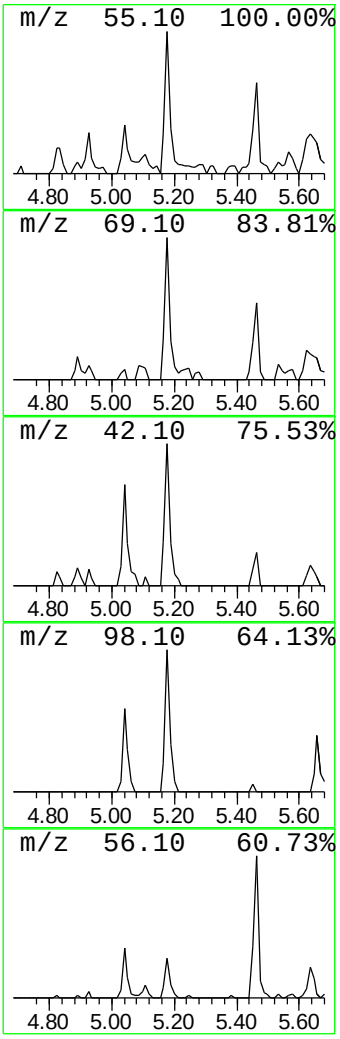
Peak Number 3 Cyclopentanone, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.38 ng	54858	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	91
2	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	91
3	1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	64
4	Cyclobutanone, 2-ethyl-	98	C6H10O	010374-14-8	53
5	Cyclohexanone	98	C6H10O	000108-94-1	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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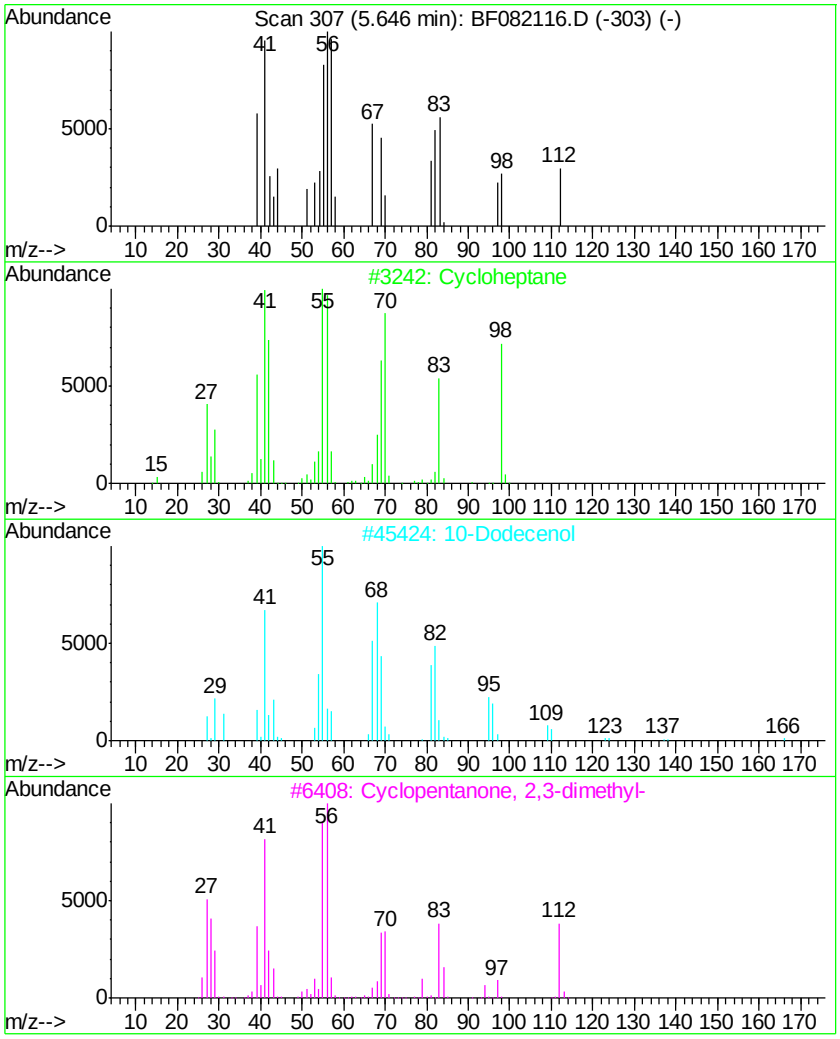
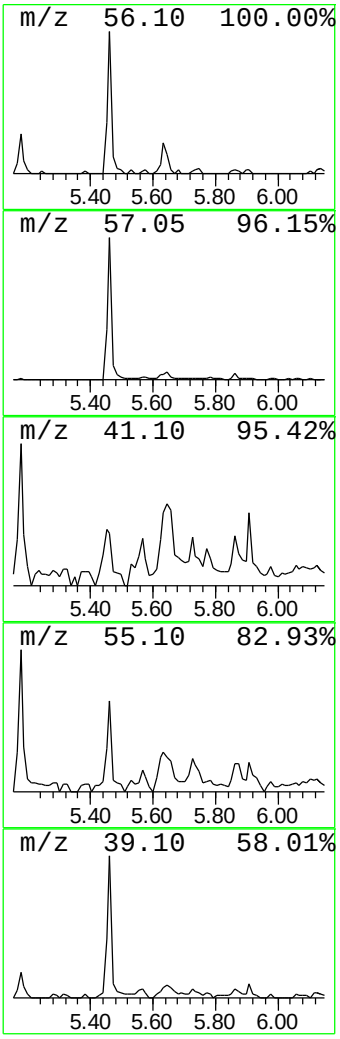
Peak Number 4 unknown5.65 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	2.32 ng	53515	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptane	98	C7H14	000291-64-5	37
2	10-Dodecenol	184	C12H24O	035237-63-9	35
3	Cyclopentanone, 2,3-dimethyl-	112	C7H12O	1000151-06-7	35
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	35
5	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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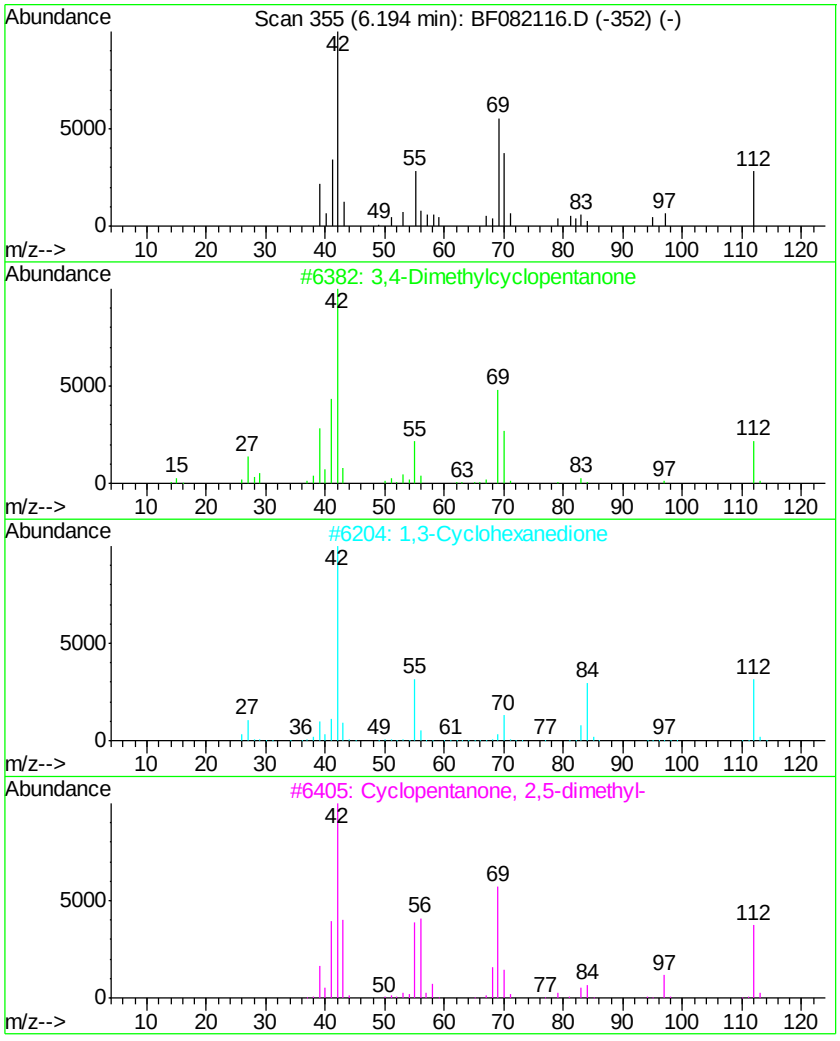
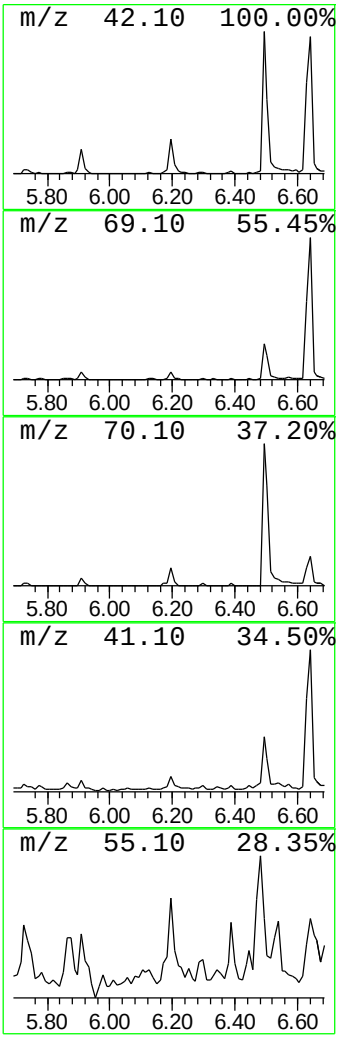
Peak Number 5 3,4-Dimethylcyclopentanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	2.24 ng	51635	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylcyclopentanone	112	C7H12O	058372-16-0	80
2	1,3-Cyclohexanedione	112	C6H8O2	000504-02-9	59
3	Cyclopentanone, 2,5-dimethyl-	112	C7H12O	004041-09-2	50
4	Cyclopentanone, 2,4-dimethyl-	112	C7H12O	001121-33-1	50
5	Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	42





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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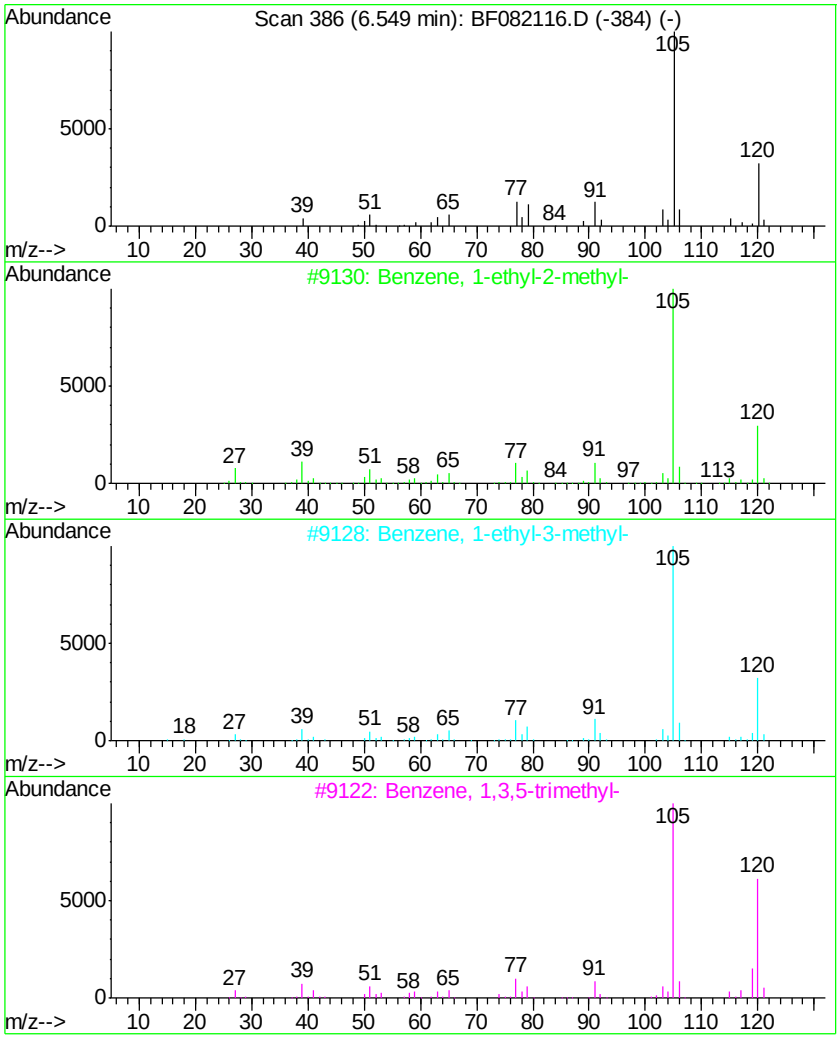
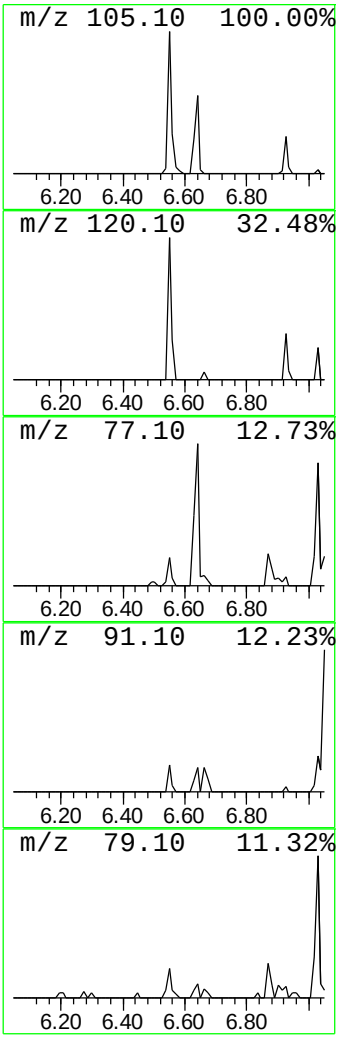
Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	3.54 ng	81463	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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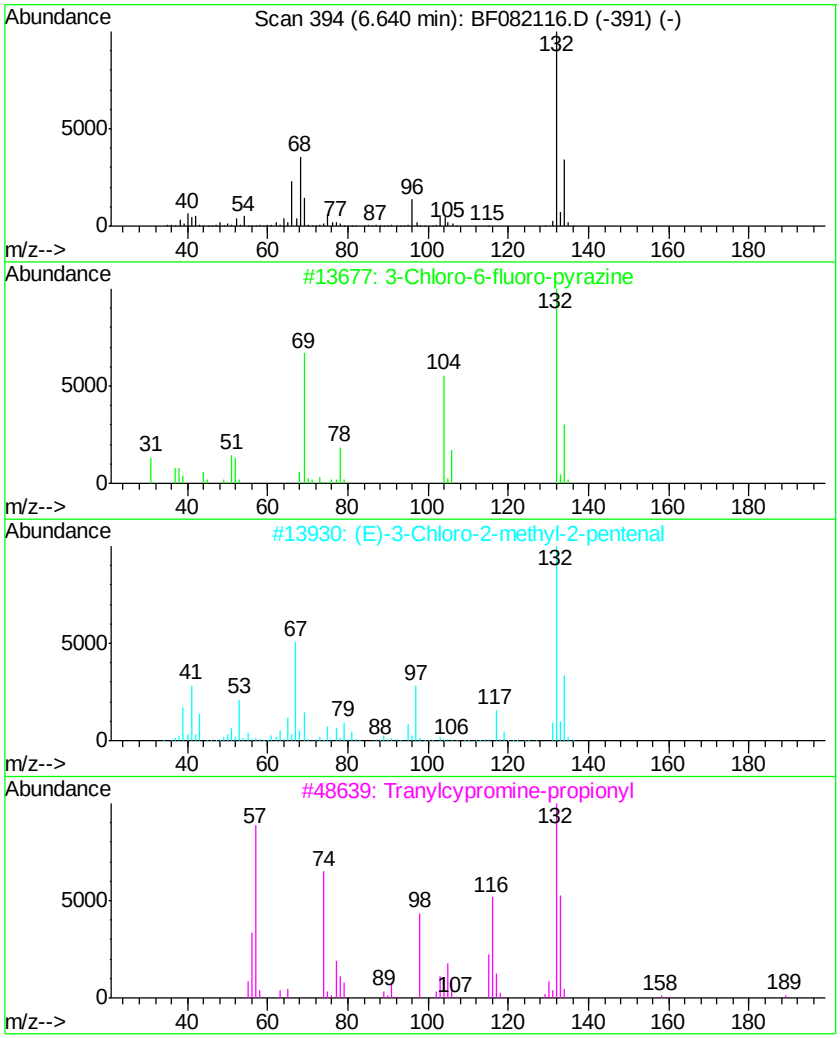
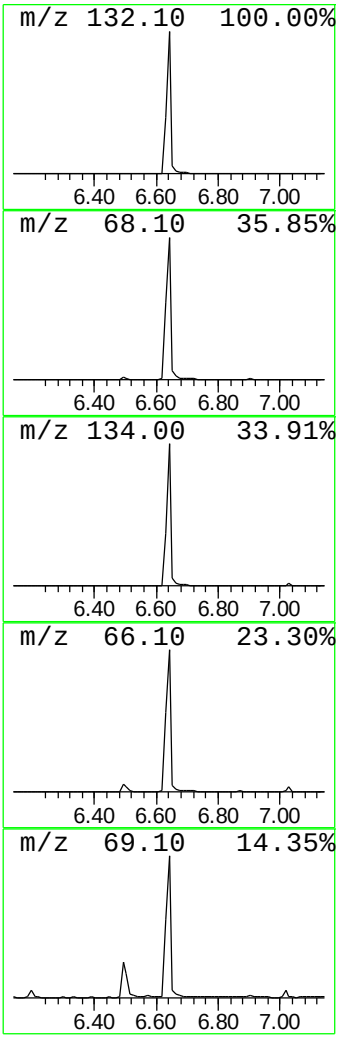
Peak Number 7 unknown6.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	86.95 ng	2003000	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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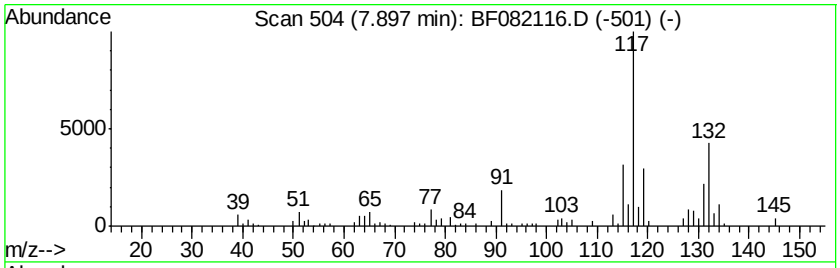
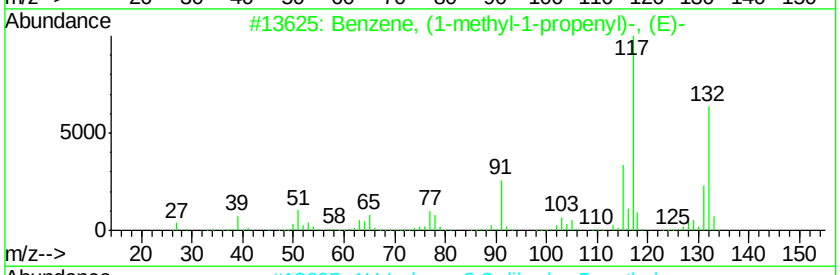
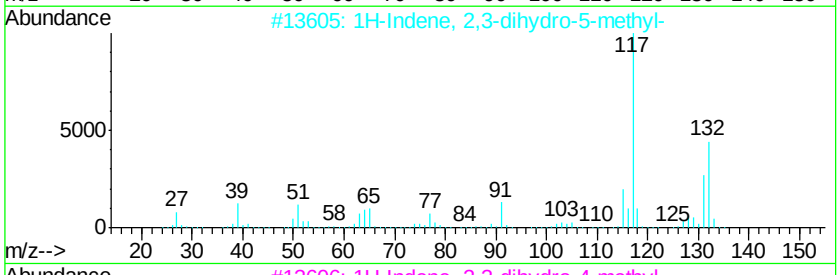
Peak Number 10 Benzene, (1-methyl-1-propen... Concentration Rank 4

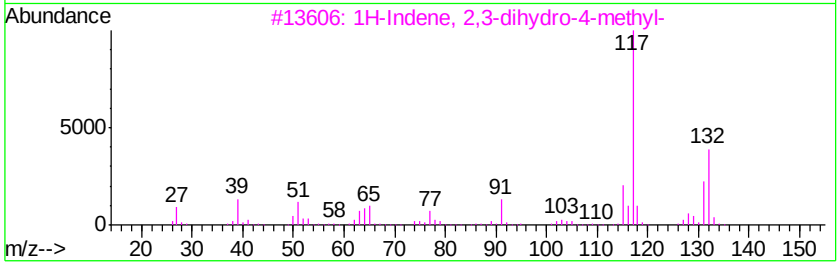
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.90	4.40 ng	163970	Naphthalene-d8	8.16

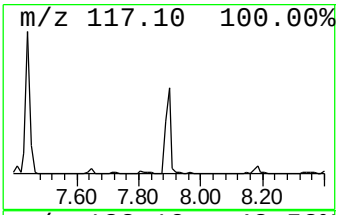
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	80
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	74

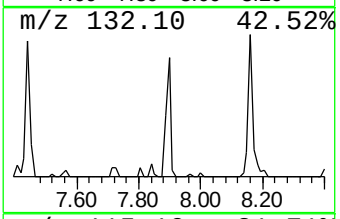


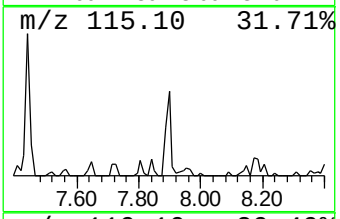


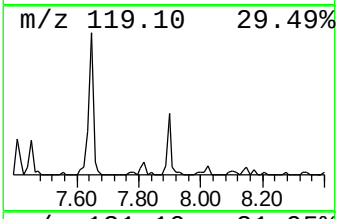


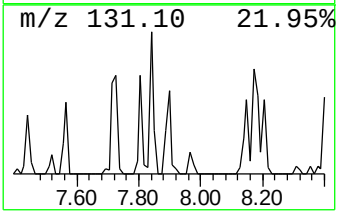












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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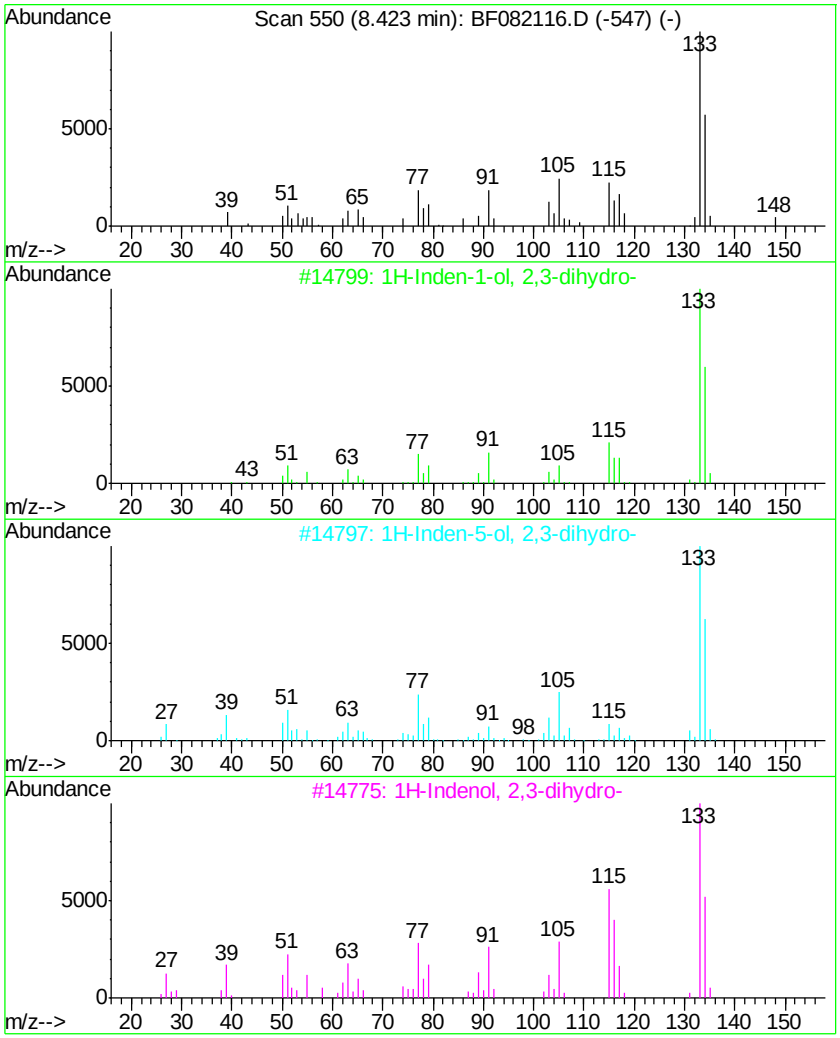
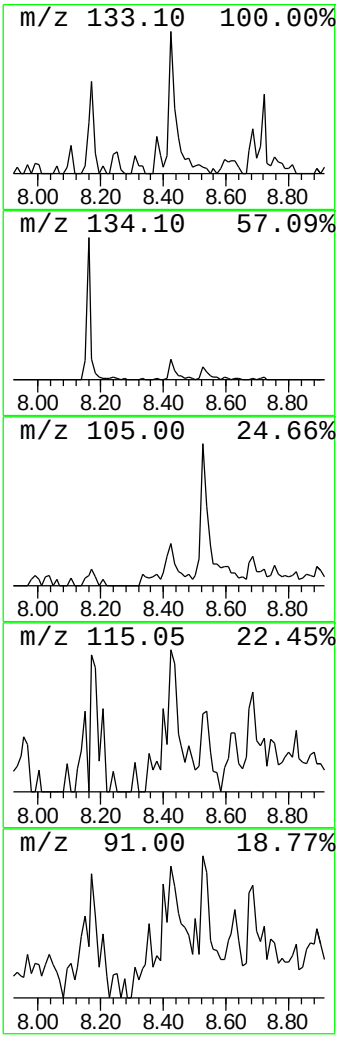
Peak Number 11 1H-Inden-1-ol, 2,3-dihydro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	2.07 ng	76934	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-ol, 2,3-dihydro-	134	C9H10O	006351-10-6	93
2	1H-Inden-5-ol, 2,3-dihydro-	134	C9H10O	001470-94-6	76
3	1H-Indenol, 2,3-dihydro-	134	C9H10O	036643-74-0	74
4	Benzaldehyde, 3,4-dimethyl-	134	C9H10O	005973-71-7	58
5	Benzaldehyde, 2,4-dimethyl-	134	C9H10O	015764-16-6	58





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Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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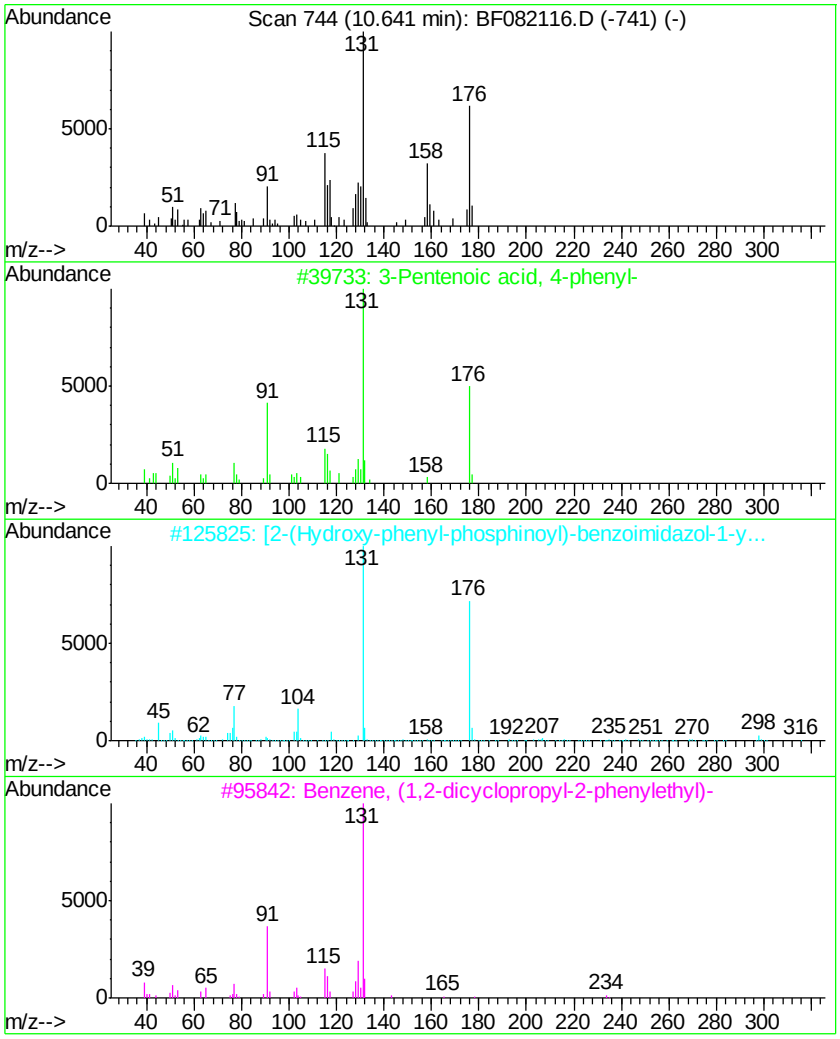
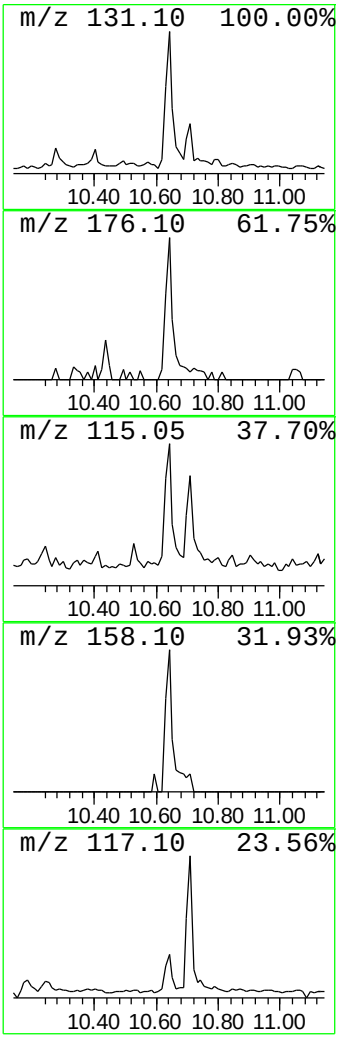
Peak Number 12 3-Pentenoic acid, 4-phenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.42 ng	94858	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	50
2	[2-(Hydroxy-phenyl-phosphinoyl)-...	316	C15H13N2O4P	300566-65-8	43
3	Benzene, (1,2-dicyclopropyl-2-ph...	262	C20H22	110330-90-0	38
4	Cyclopropane, 2-bromo-1-methyl-1...	210	C10H11Br	055091-64-0	38
5	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	38





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Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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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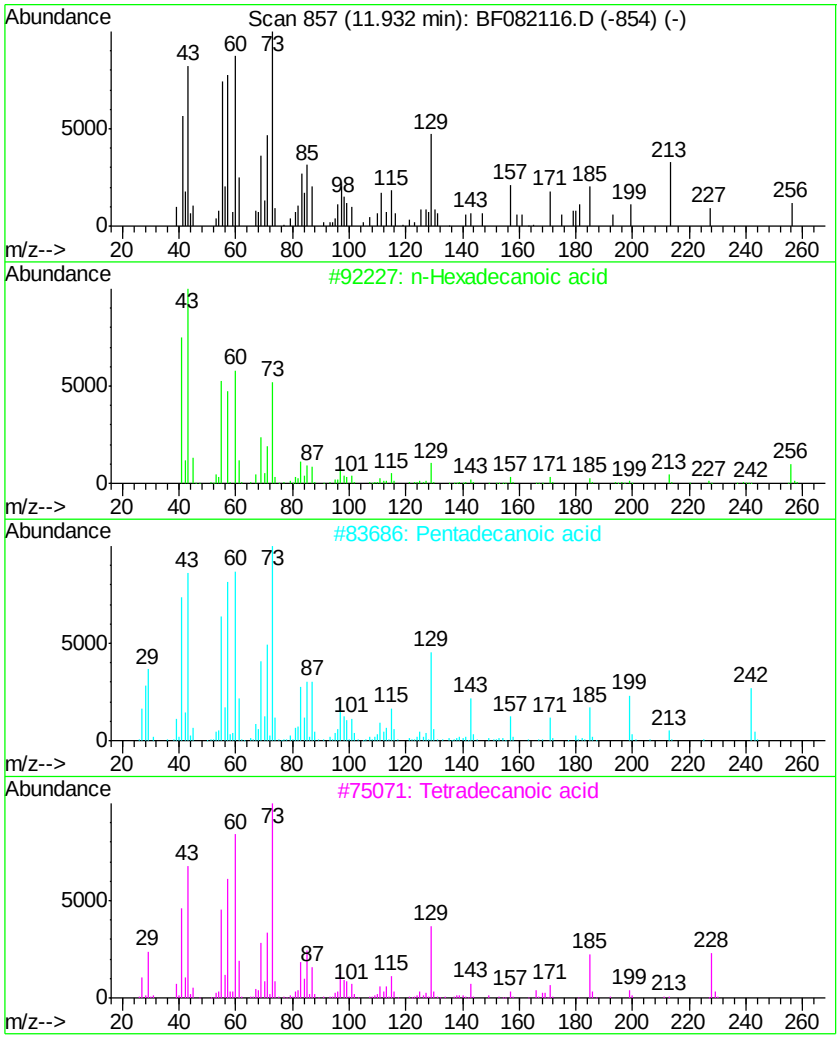
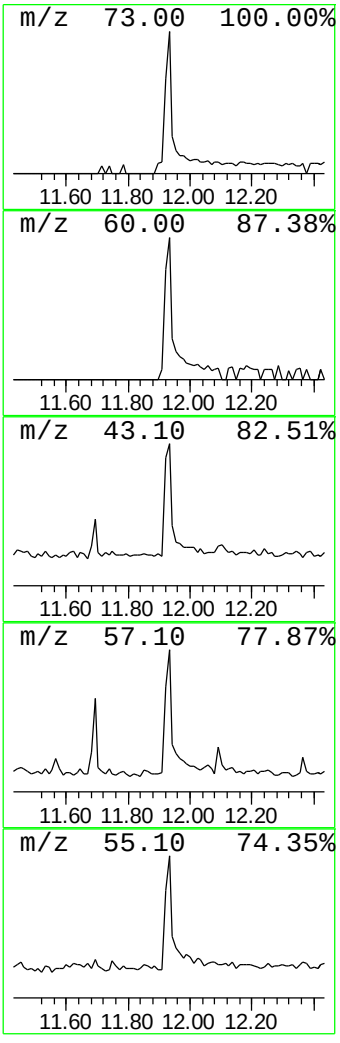
Peak Number 13 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.43 ng	91148	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
Data File : BF082116.D
Acq On : 7 Oct 2015 21:05
Operator : UM/IZ
Sample : G3891-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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
Butanal, 2-ethyl-	4.82	2.1	ng	47395	1	6.87	460713	20.0
2-Pentanone, 4-hy...	5.04	14.4	ng	330874	1	6.87	460713	20.0
Cyclopentanone, 3...	5.18	2.4	ng	54858	1	6.87	460713	20.0
unknown5.65	5.65	2.3	ng	53515	1	6.87	460713	20.0
3,4-Dimethylcyclo...	6.19	2.2	ng	51635	1	6.87	460713	20.0
Benzene, 1-ethyl-...	6.55	3.5	ng	81463	1	6.87	460713	20.0
unknown6.64	6.64	87.0	ng	2003000	1	6.87	460713	20.0
Benzene, (1-methy...	7.90	4.4	ng	163970	2	8.16	744813	20.0
1H-Inden-1-ol, 2,...	8.42	2.1	ng	76934	2	8.16	744813	20.0
3-Pentenoic acid,...	10.64	2.4	ng	94858	3	9.92	783424	20.0
n-Hexadecanoic acid	11.93	2.4	ng	91148	4	11.41	750452	20.0