LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081289.D
Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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-BF081715.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	2.994	105	110	114	rBV	735762	1334351	4.07%	2.381%
2	5.051	287	290	298	rVB	585249	746810	2.28%	1.332%
3	6.000	362	373	374	rBV2	5987433	32824305	100.00%	58.562%
4	6.149	383	386	390	rBV2	394225	770209	2.35%	1.374%
5	6.252	394	395	398	rVV	1009353	1075242	3.28%	1.918%
6	6.480	413	415	417	rBV	442016	393466	1.20%	0.702%
7	6.537	417	420	426	rVB2	244862	432036	1.32%	0.771%
8	6.640	426	429	430	rBV	1290479	1158042	3.53%	2.066%
9	7.052	462	465	468	rVV	801864	1042608	3.18%	1.860%
10	7.772	525	528	529	rVV	488241	514040	1.57%	0.917%
11	8.160	556	562	564	rBV3	161665	591242	1.80%	1.055%
12	8.206	564	566	568	rVV2	306978	631732	1.92%	1.127%
13	8.252	568	570	572	rVV	335810	508683	1.55%	0.908%
14	8.343	574	578	581	rVV3	503924	1079750	3.29%	1.926%
15	8.435	584	586	587	rVV	230635	346955	1.06%	0.619%
16	8.480	587	590	593	rVV	334891	694548	2.12%	1.239%
17	8.652	601	605	611	rBV2	234216	713755	2.17%	1.273%
18	8.858	616	623	625	rBV	1621771	3133369	9.55%	5.590%
19	9.509	678	680	684	rVB	571061	588134	1.79%	1.049%
20	9.841	704	709	711	rVV4	163780	477267	1.45%	0.851%
21	9.955	714	719	722	rVB	211840	503644	1.53%	0.899%
22	10.298	746	749	751	rVB	993123	969316	2.95%	1.729%
23	10.983	805	809	811	rBV	560584	648709	1.98%	1.157%
24	11.555	857	859	861	rBV	399780	426107	1.30%	0.760%
25	12.001	895	898	900	rBV	365282	410502	1.25%	0.732%
26	12.172	909	913	914	rBV	743141	1213331	3.70%	2.165%
27	12.332	925	927	932	rVB	566622	575102	1.75%	1.026%
28	12.572	945	948	950	rBV	1057070	1445728	4.40%	2.579%
29	13.589	1035	1037	1040	rVB	373358	374607	1.14%	0.668%
30	14.972	1155	1158	1161	rVB	370674	427257	1.30%	0.762%

Sum of corrected areas: 56050847

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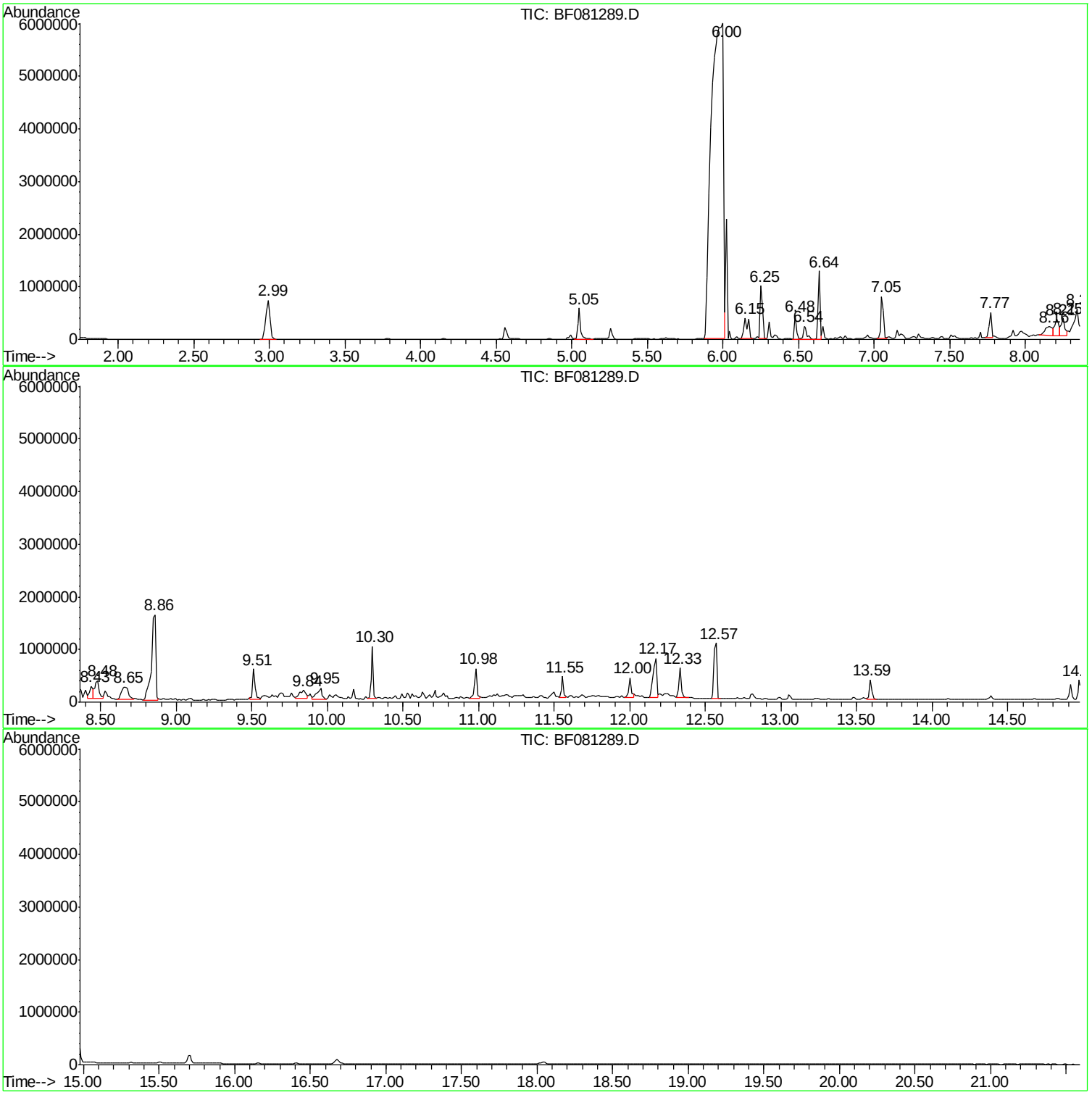
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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

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Data File : BF081289.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

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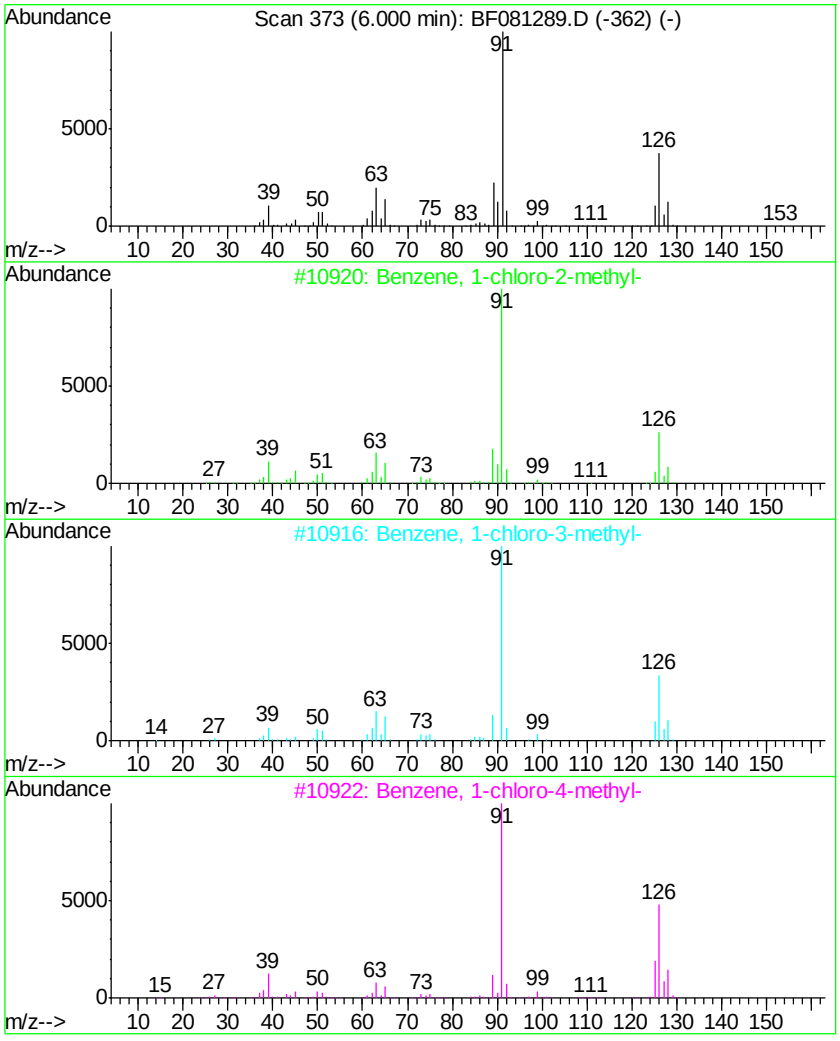
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

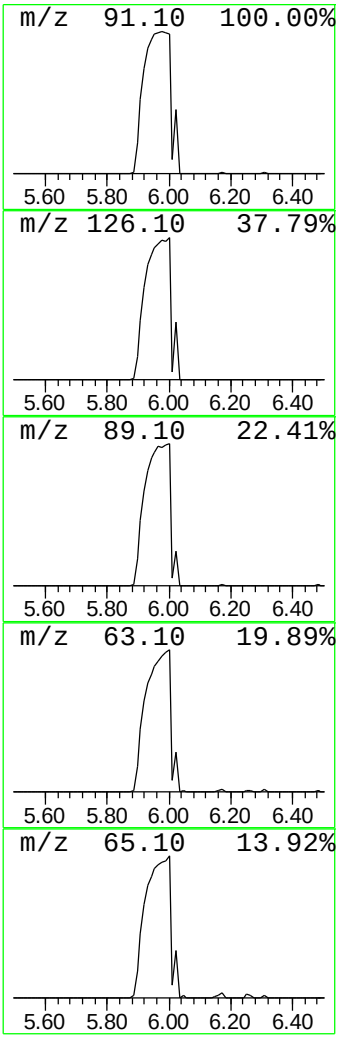
****

Peak Number 2 Benzene, 1-chloro-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	1668.47 ng	32824300	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	96
2	Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	95
3	Benzene, 1-chloro-4-methyl-	126	C7H7Cl	000106-43-4	87
4	Benzyl chloride	126	C7H7Cl	000100-44-7	62
5	Benzenemethanesulfonyl chloride	190	C7H7ClO2S	001939-99-7	40





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Data File : BF081289.D
Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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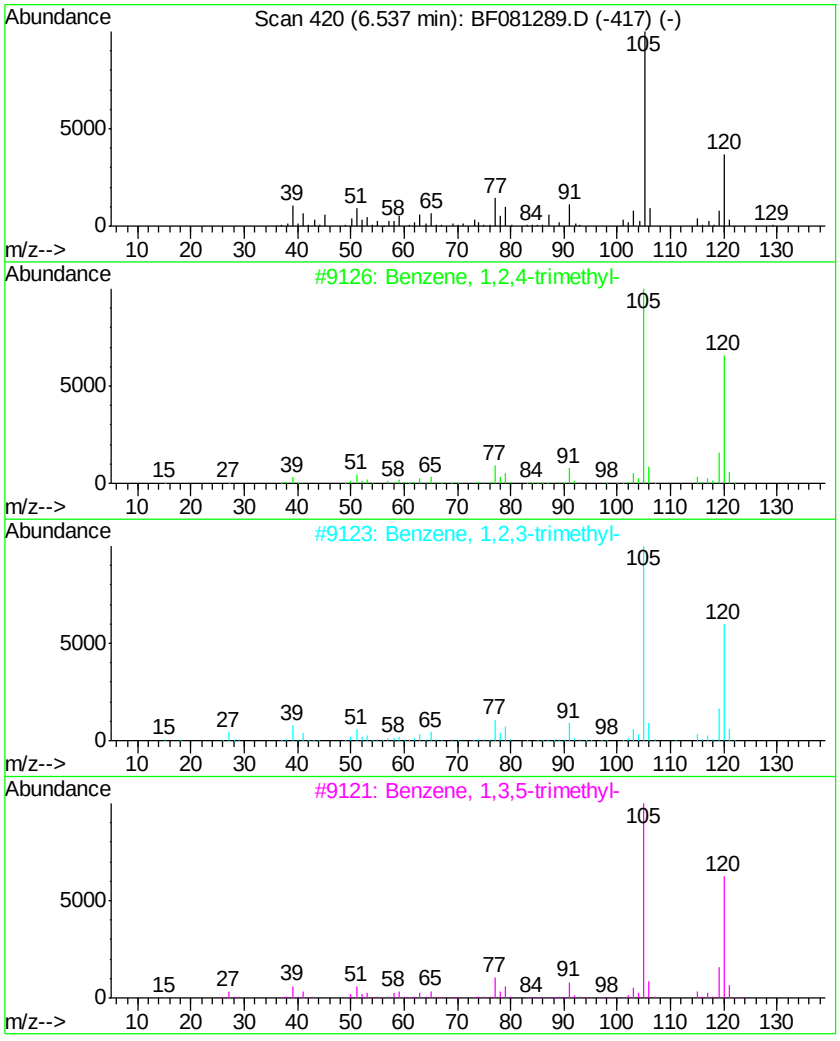
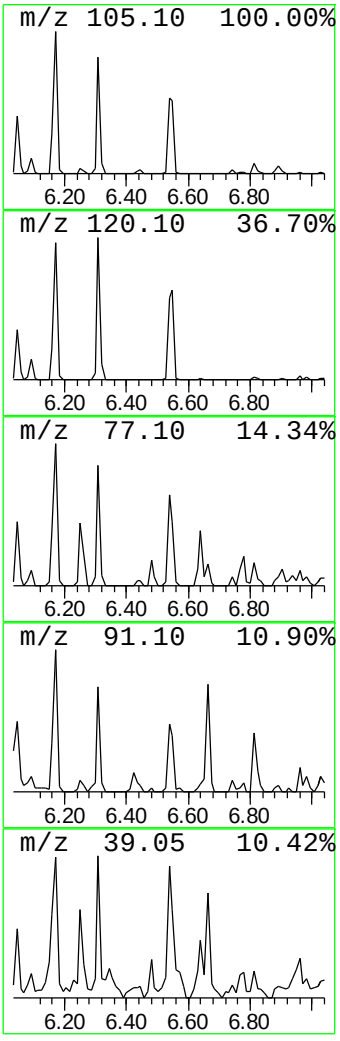
Peak Number 4 Benzene, 1,2,4-trimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	21.96 ng	432036	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081289.D
Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

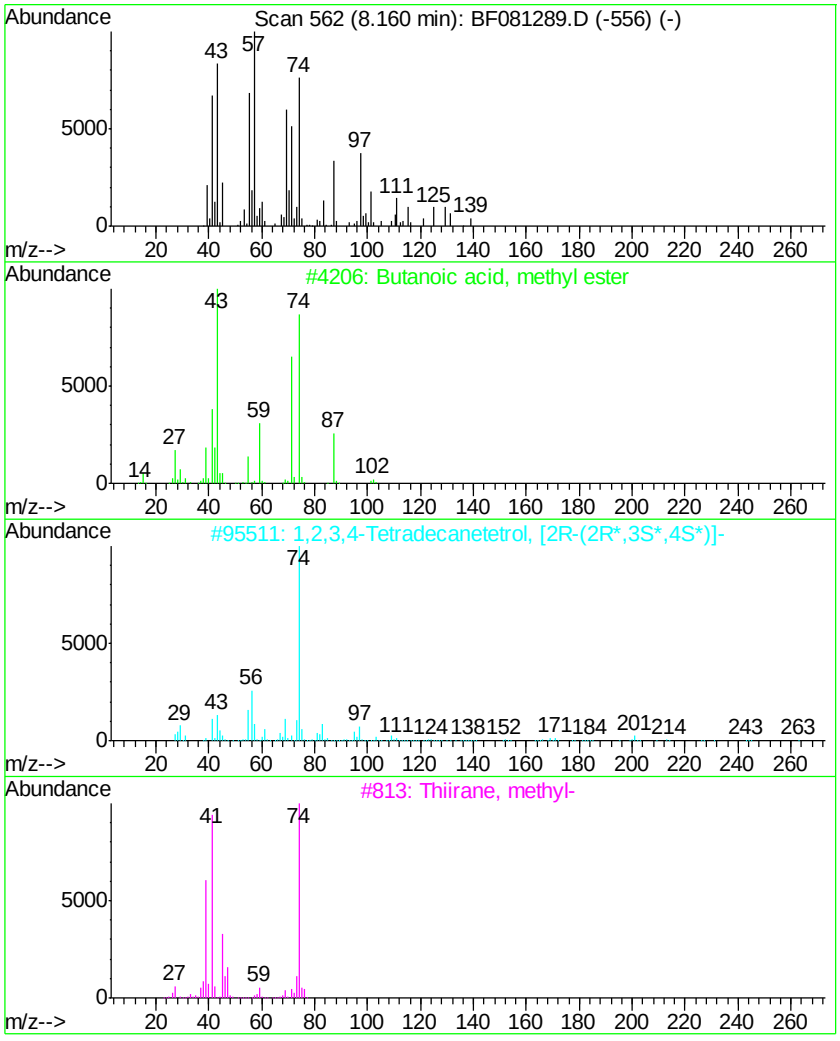
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

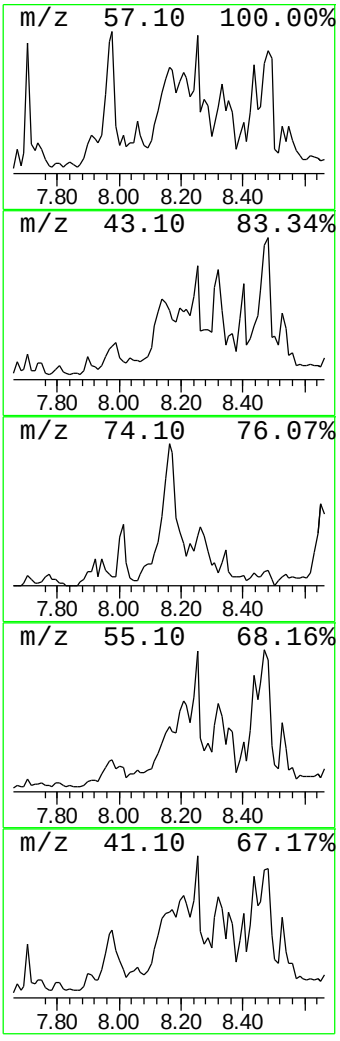
****

Peak Number 6 unknown8.16 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	23.00 ng	591242	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	47
2	1,2,3,4-Tetradecanetetrol, [2R-(...	262	C14H30O4	136953-04-3	35
3	Thiirane, methyl-	74	C3H6S	001072-43-1	27
4	Allyl mercaptan	74	C3H6S	000870-23-5	27
5	Methyl 4-hydroxybutanoate	118	C5H10O3	000925-57-5	25





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Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

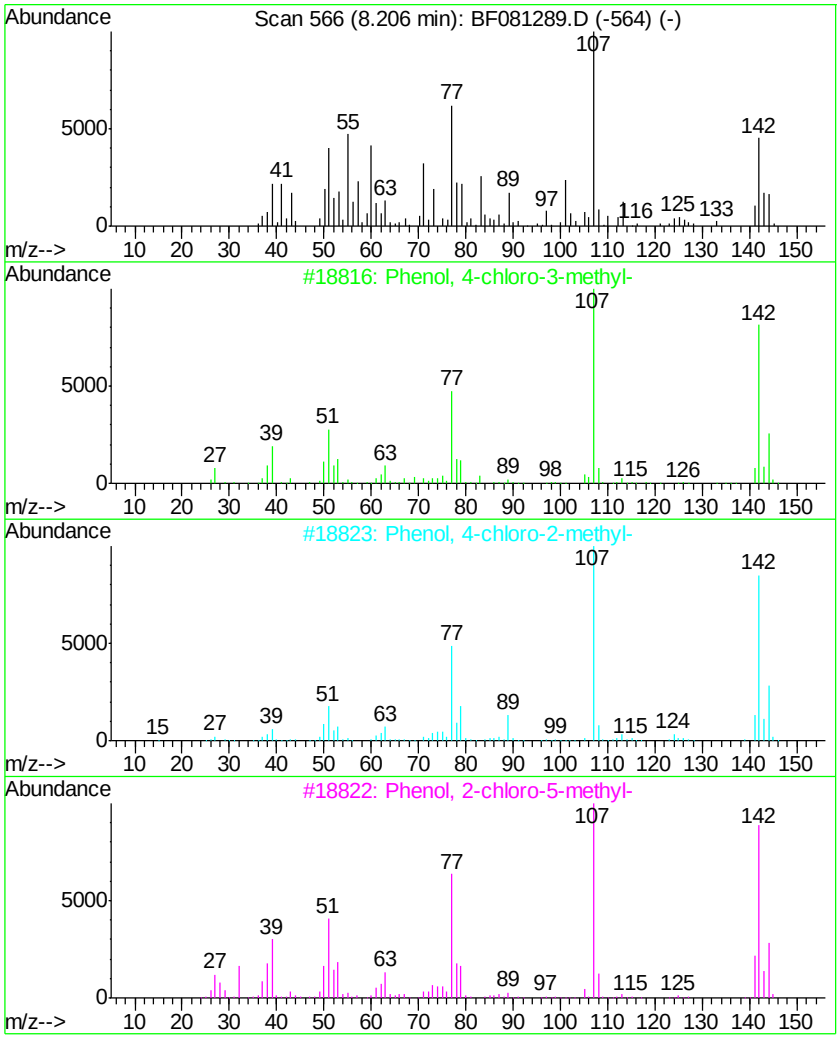
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

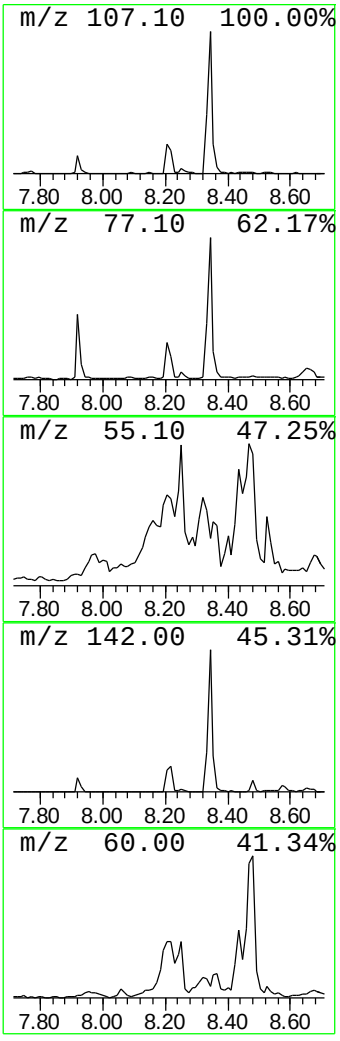
****

Peak Number 7 Phenol, 4-chloro-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.21	24.58 ng	631732	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-chloro-3-methyl-	142	C7H7ClO	000059-50-7	94
2	Phenol, 4-chloro-2-methyl-	142	C7H7ClO	001570-64-5	89
3	Phenol, 2-chloro-5-methyl-	142	C7H7ClO	000615-74-7	76
4	Phenol, 2-chloro-6-methyl-	142	C7H7ClO	000087-64-9	70
5	Phenol, 2-chloro-4-methyl-	142	C7H7ClO	006640-27-3	70





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081289.D
Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

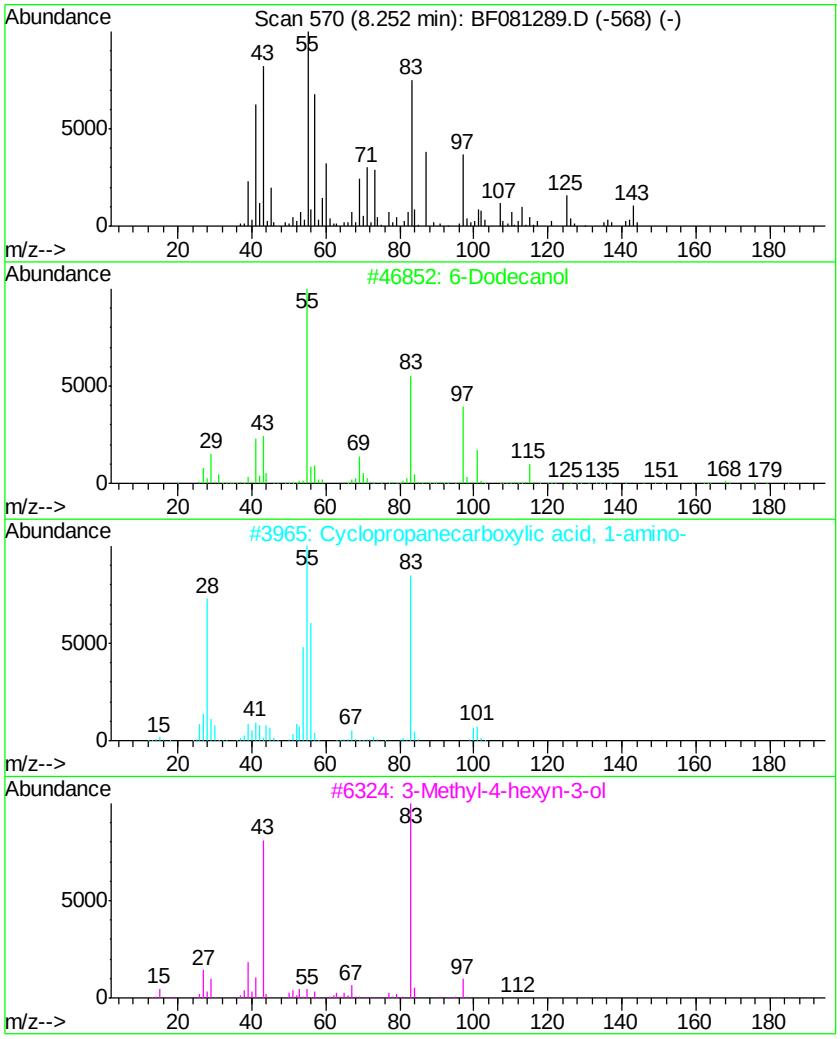
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

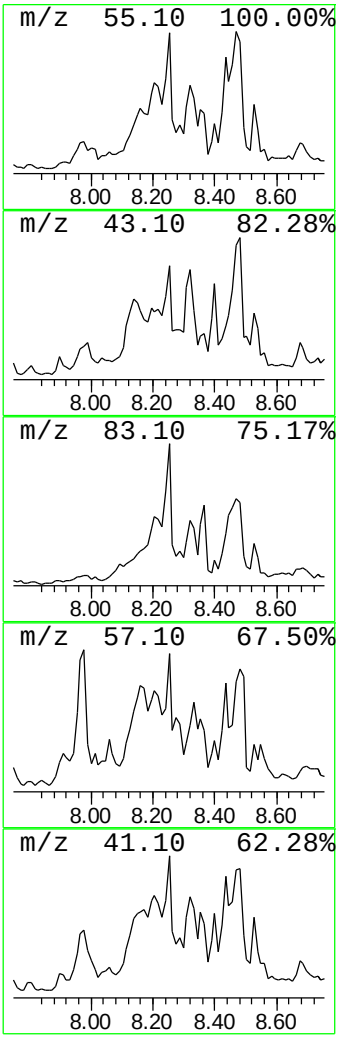
****

Peak Number 8 unknown8.25 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	19.79 ng	508683	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Dodecanol	186	C12H26O	006836-38-0	27
2	Cyclopropanecarboxylic acid, 1-a...	101	C4H7NO2	022059-21-8	22
3	3-Methyl-4-hexyn-3-ol	112	C7H12O	006320-68-9	22
4	Bis(2-ethylhexyl) hydrogen phosp...	306	C16H35O3P	003658-48-8	16
5	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	16





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Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

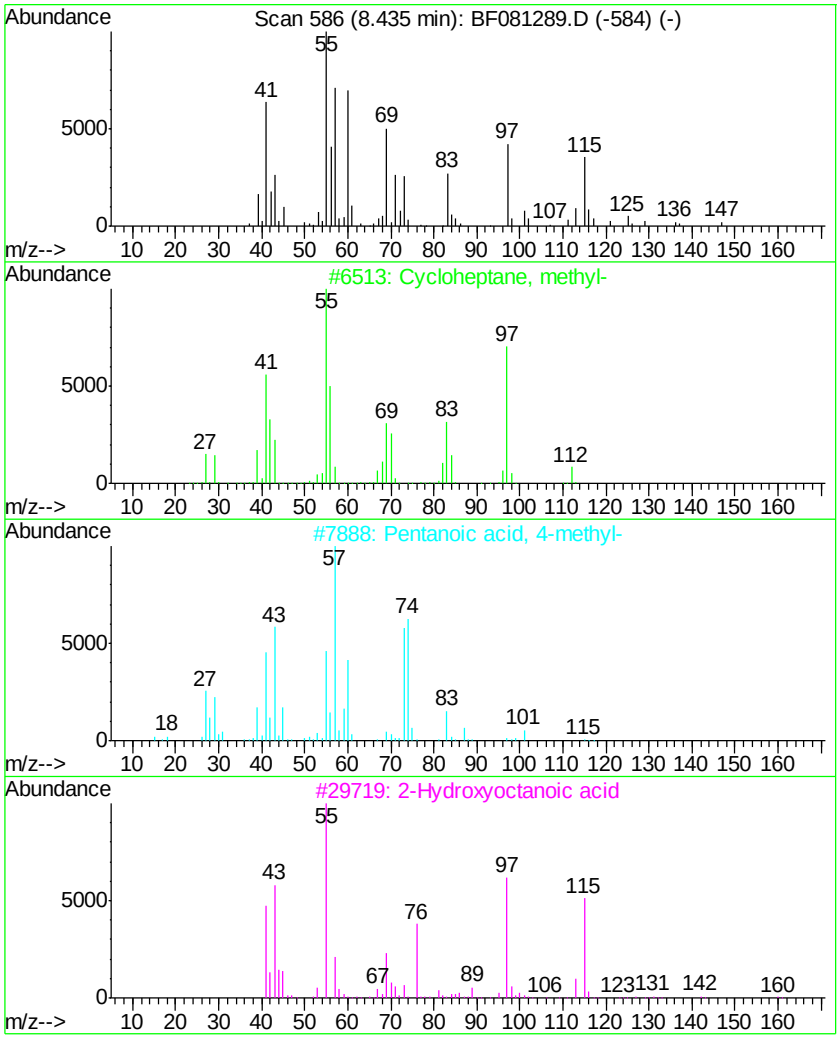
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

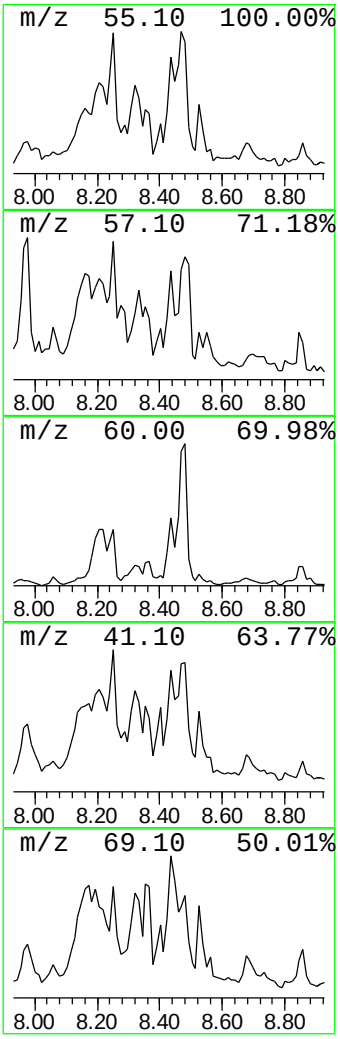
****

Peak Number 9 unknown8.43 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	13.50 ng	346955	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptane, methyl-	112	C8H16	004126-78-7	32
2	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	17
3	2-Hydroxyoctanoic acid	160	C8H16O3	000617-73-2	16
4	Hexanoic acid	116	C6H12O2	000142-62-1	14
5	2-Methyl-1-undecanol	186	C12H26O	010522-26-6	12





Library Search Compound Report

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Operator : UM/IZ
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Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

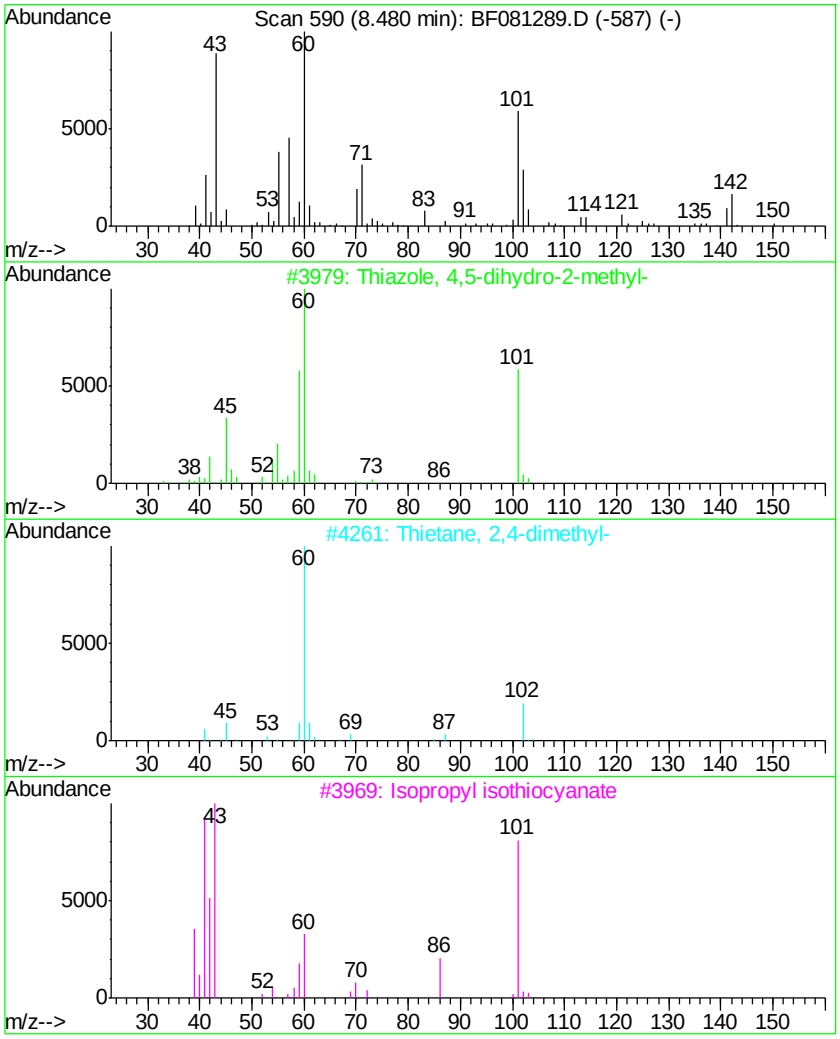
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

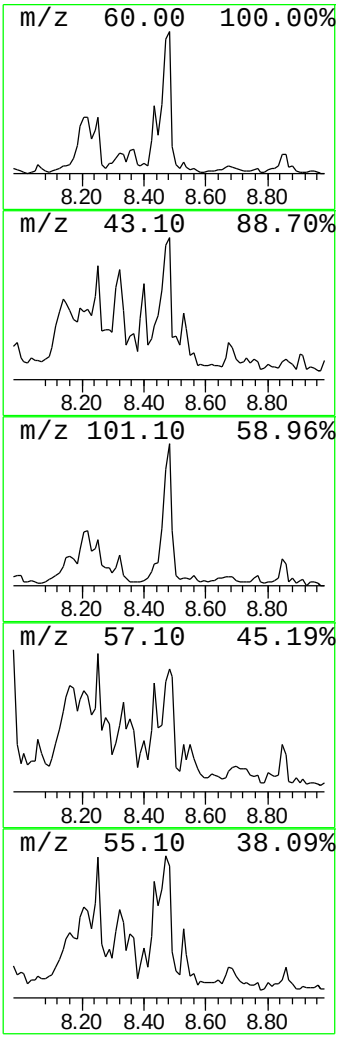
****

Peak Number 10 Thiazole, 4,5-dihydro-2-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	27.02 ng	694548	Naphthalene-d8	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	50
2	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	37
3	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	37
4	Methyl .beta.-d-galactopyranoside	194	C7H14O6	1000126-04-6	23
5	Cyclopentaneacetic acid	128	C7H12O2	001123-00-8	10





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

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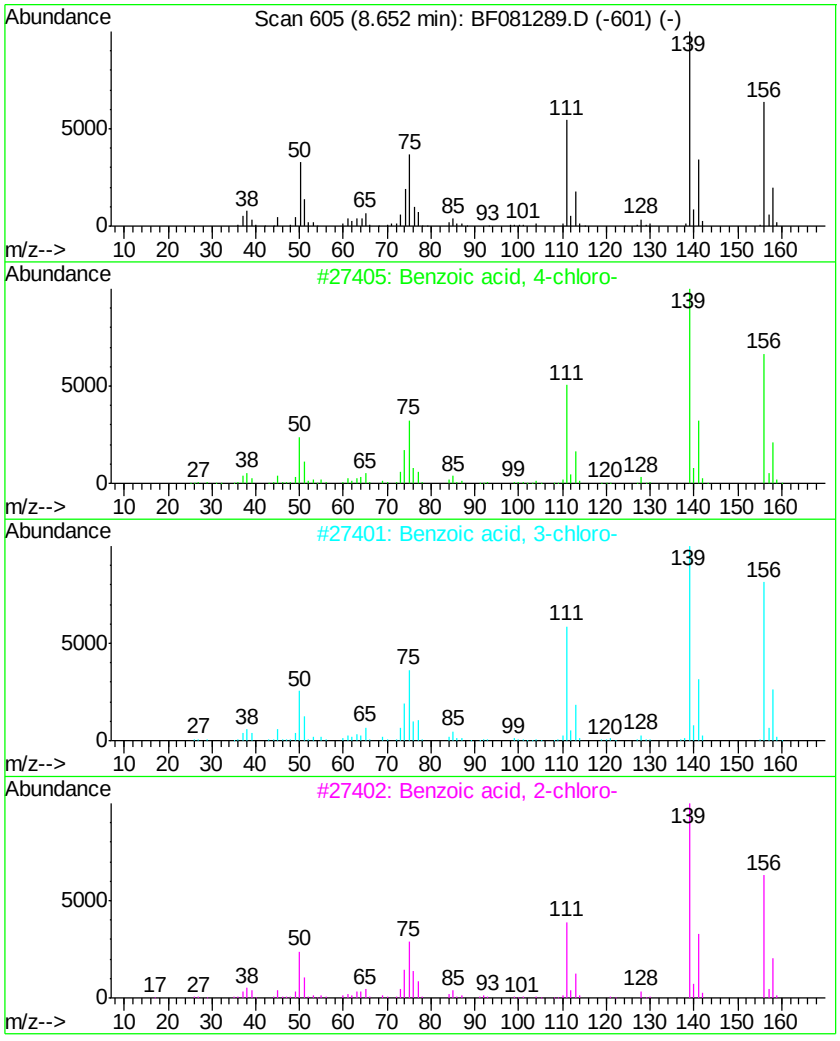
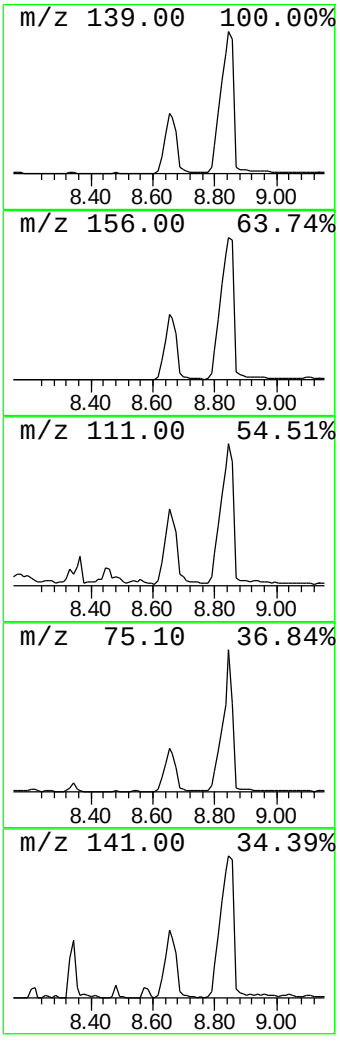
Peak Number 11 Benzoic acid, 4-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	24.27 ng	713755	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-chloro-	156	C7H5ClO2	000074-11-3	98
2	Benzoic acid, 3-chloro-	156	C7H5ClO2	000535-80-8	98
3	Benzoic acid, 2-chloro-	156	C7H5ClO2	000118-91-2	94
4	Acetic acid, 2-(4-chlorobenzoyla...	289	C15H12ClNO3	028172-56-7	81
5	Ethanone, 1-(4-chlorophenyl)-	154	C8H7ClO	000099-91-2	72





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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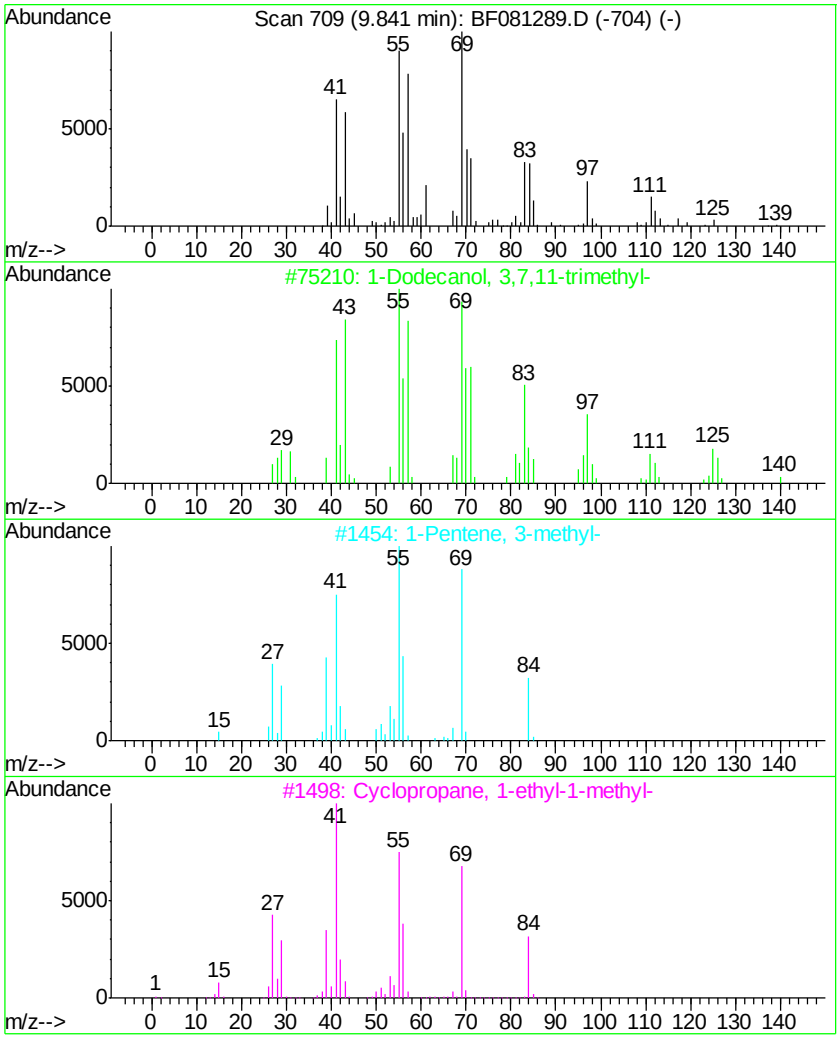
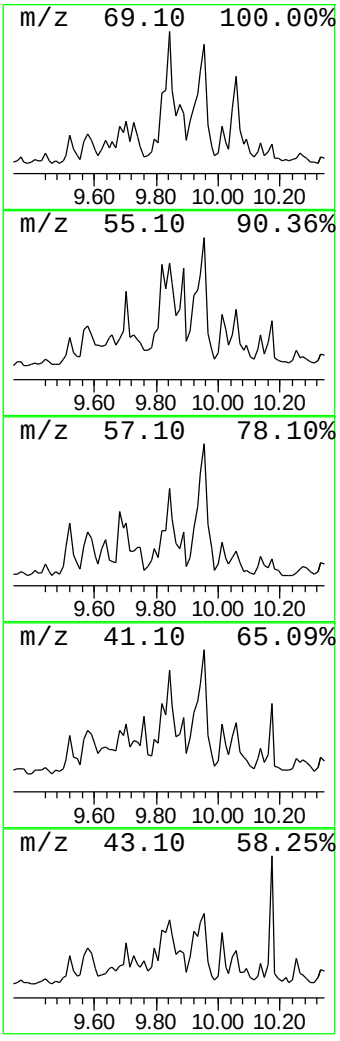
Peak Number 12 unknown9.84 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	16.23 ng	477267	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	43
2	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	38
3	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	38
4	Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	38
5	Isooctanol	130	C8H18O	026952-21-6	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
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Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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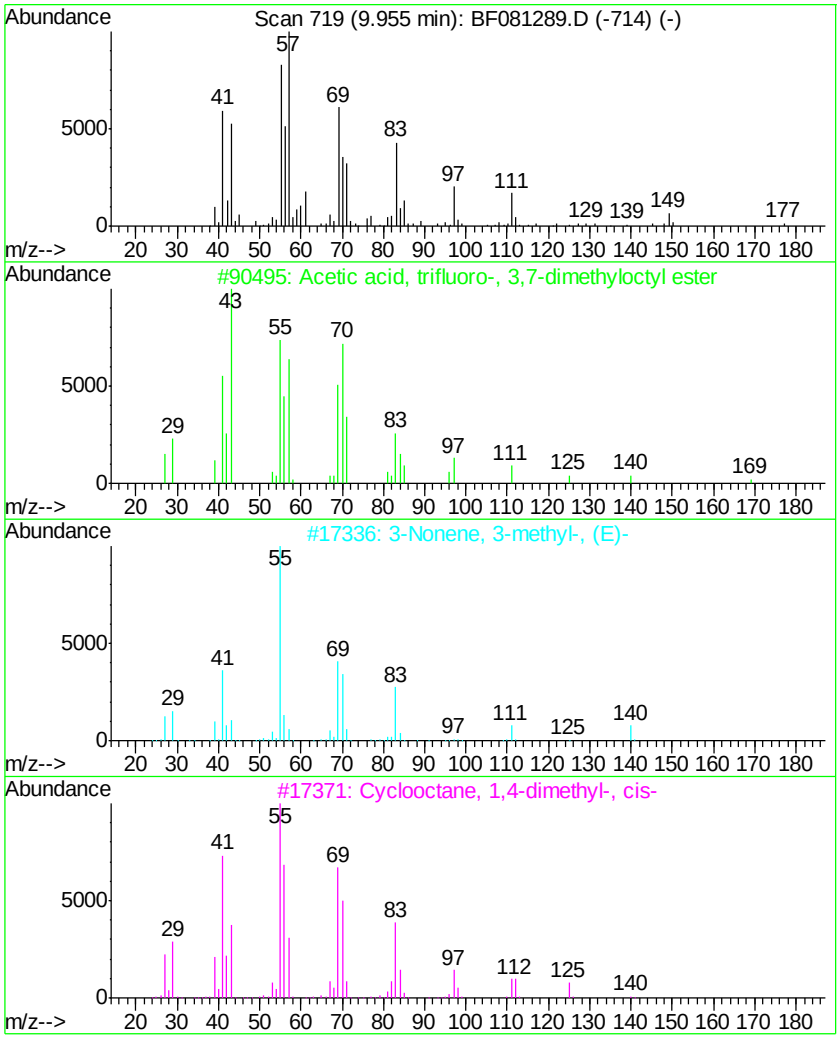
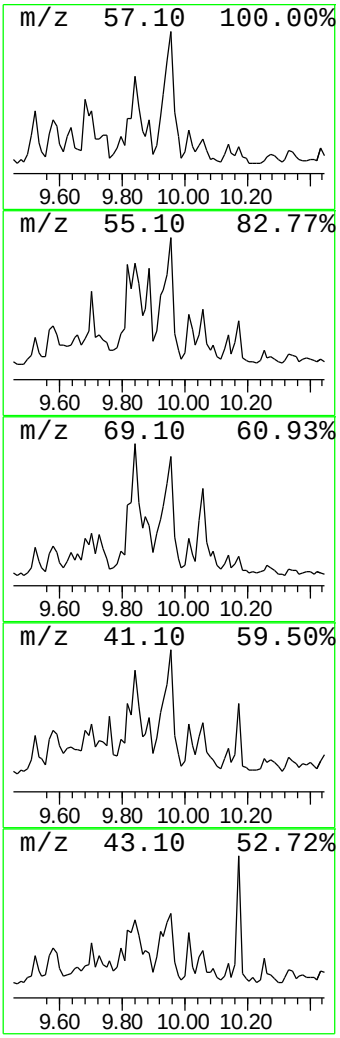
Peak Number 13 unknown9.95 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.95	17.13 ng	503644	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, trifluoro-, 3,7-dim...	254	C12H21F3O2	028745-07-5	43
2	3-Nonene, 3-methyl-, (E)-	140	C10H20	069405-42-1	38
3	Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	38
4	4-Nonene, 5-methyl-	140	C10H20	015918-07-7	38
5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082915\
Data File : BF081289.D
Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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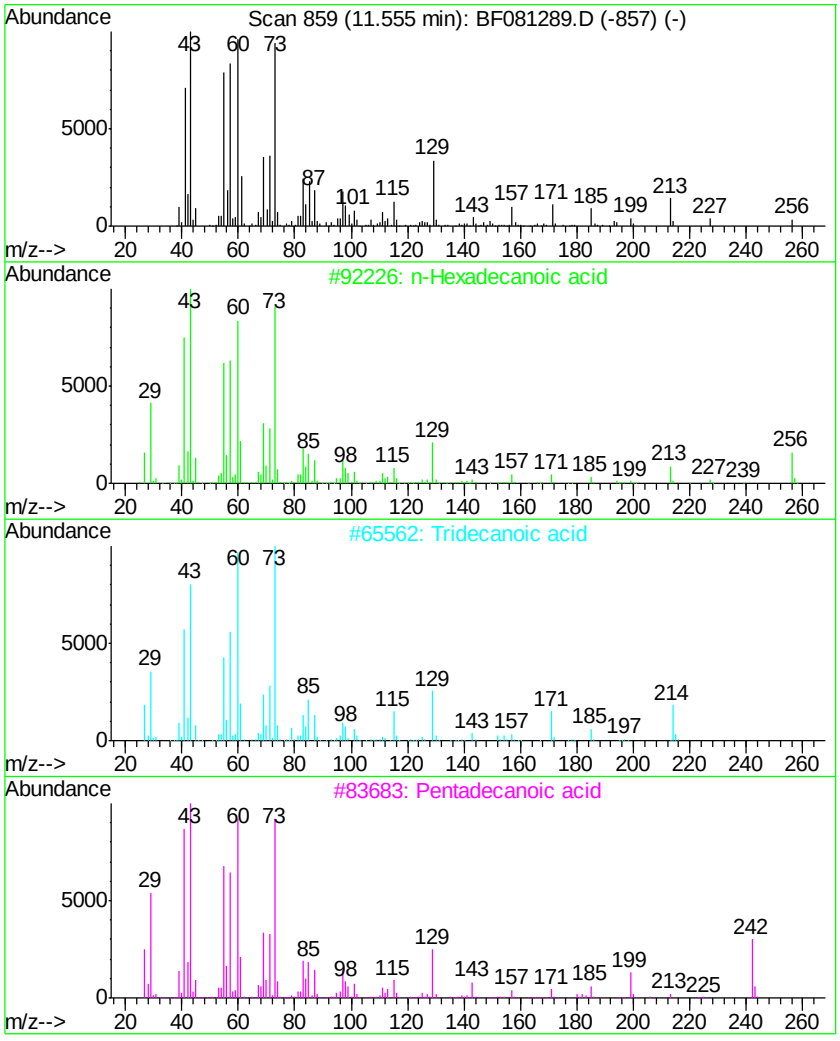
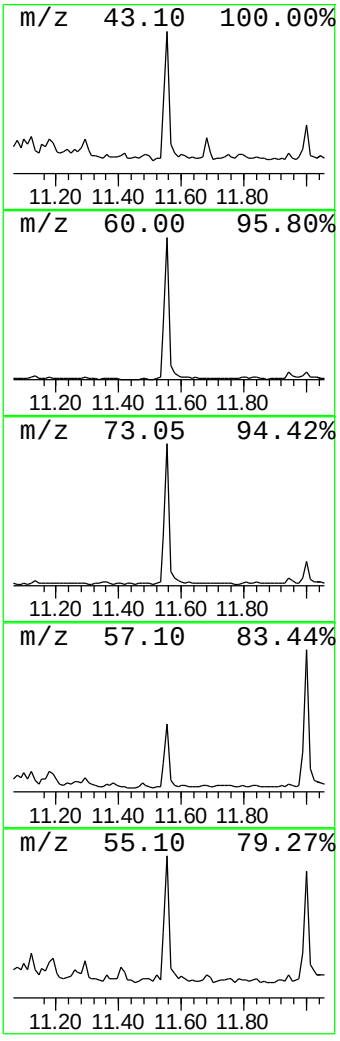
Peak Number 14 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	13.14 ng	426107	Phenanthrene-d10	10.98

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	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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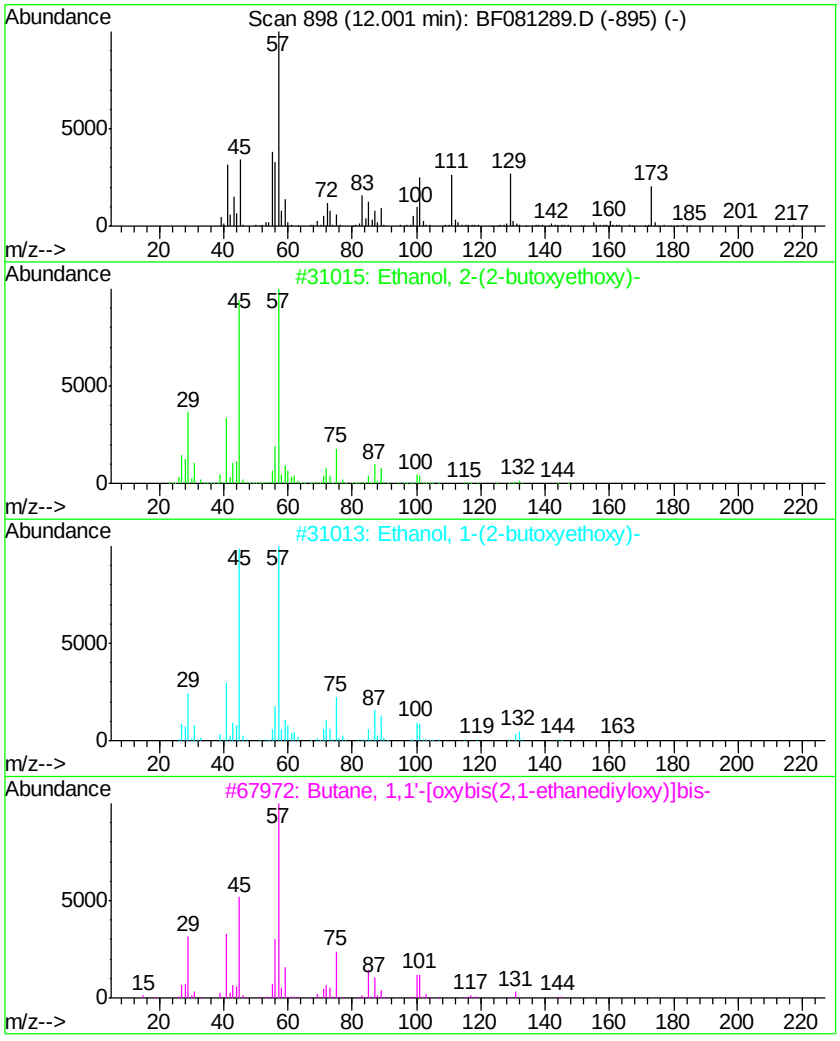
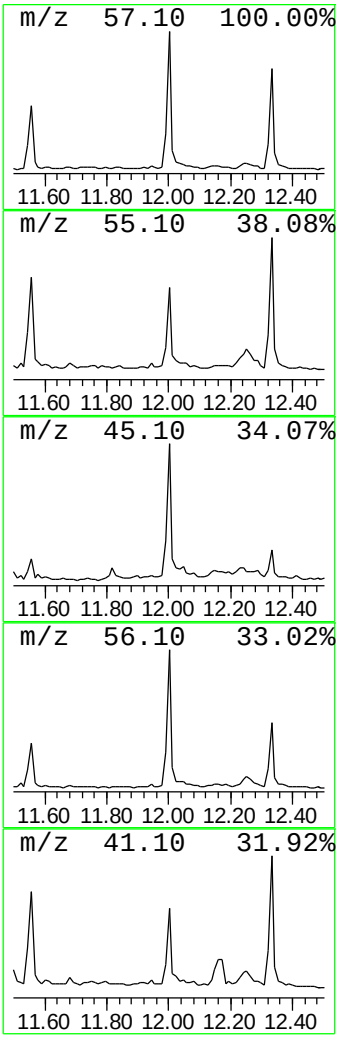
Peak Number 15 unknown12.00 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	12.66 ng	410502	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	25
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	25
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	22
4	6-Dodecanone, 5,8-diethyl-7-hydr...	256	C16H32O2	031814-59-2	16
5	N.alpha.-(tert-butoxycarbonyl)gl...	367	C16H21N3O7	1000224-55-0	16





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Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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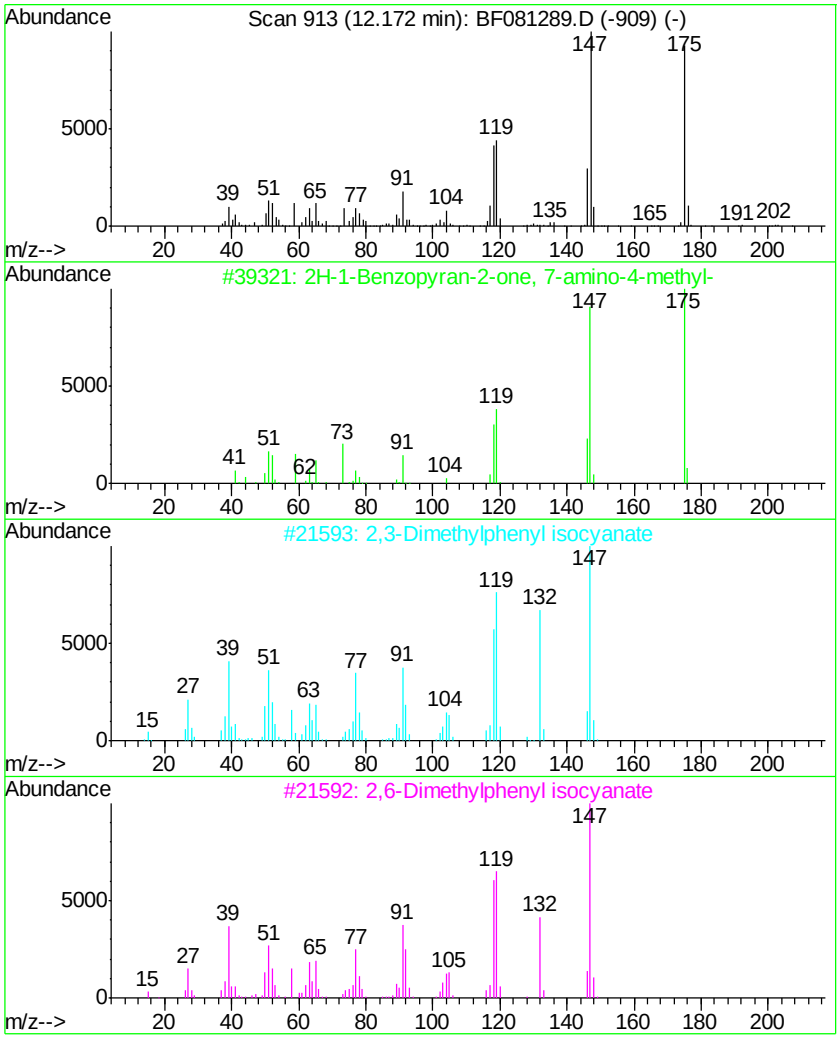
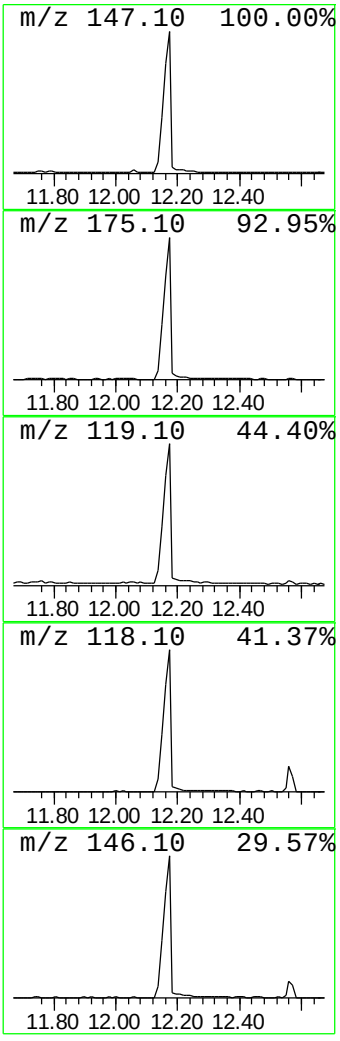
Peak Number 16 2H-1-Benzopyran-2-one, 7-am... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	37.41 ng	1213330	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1-Benzopyran-2-one, 7-amino-4...	175	C10H9NO2	026093-31-2	94
2	2,3-Dimethylphenyl isocyanate	147	C9H9NO	001591-99-7	60
3	2,6-Dimethylphenyl isocyanate	147	C9H9NO	028556-81-2	53
4	(2-Benzimidazolyl)methylamine	147	C8H9N3	005805-57-2	49
5	1H-Inden-1-one, 5-amino-2,3-dihy...	147	C9H9NO	003470-54-0	46





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Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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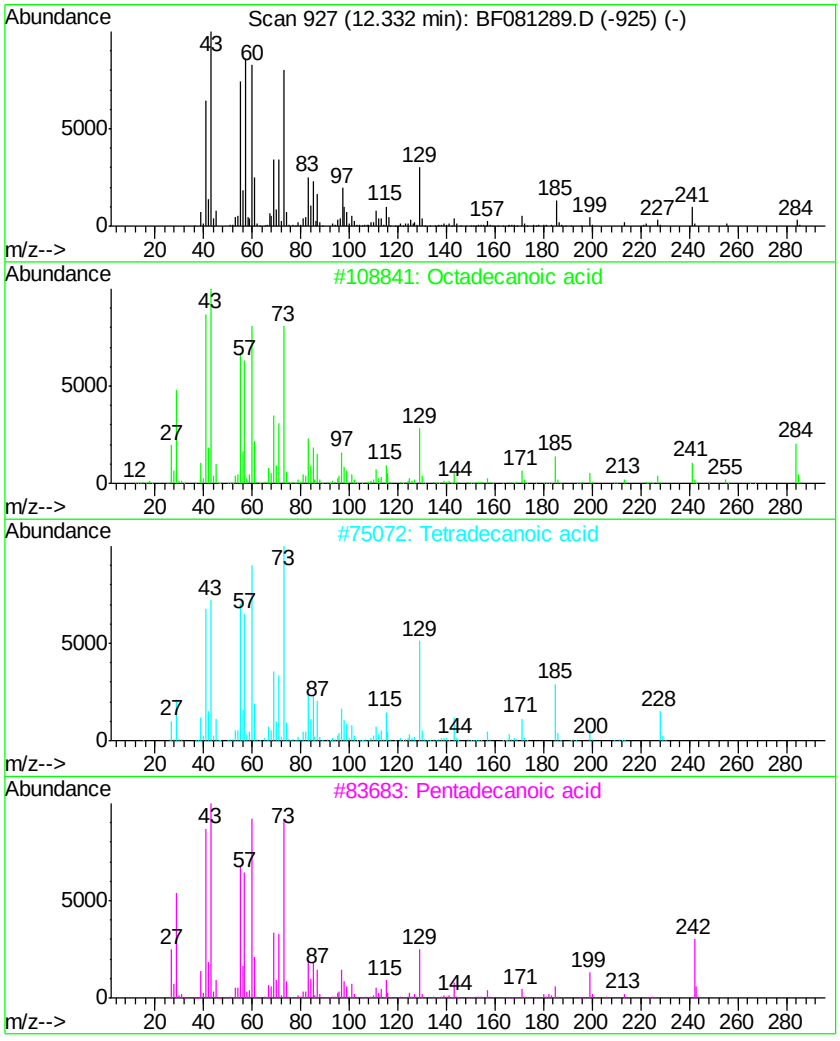
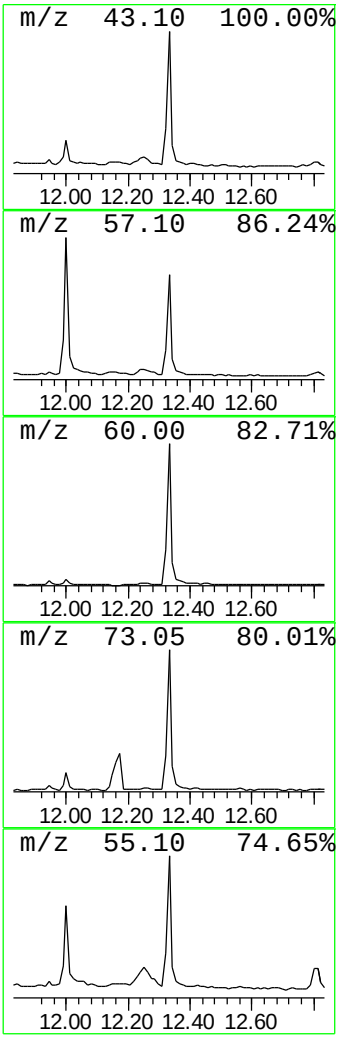
Peak Number 17 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	30.70 ng	575102	Chrysene-d12	13.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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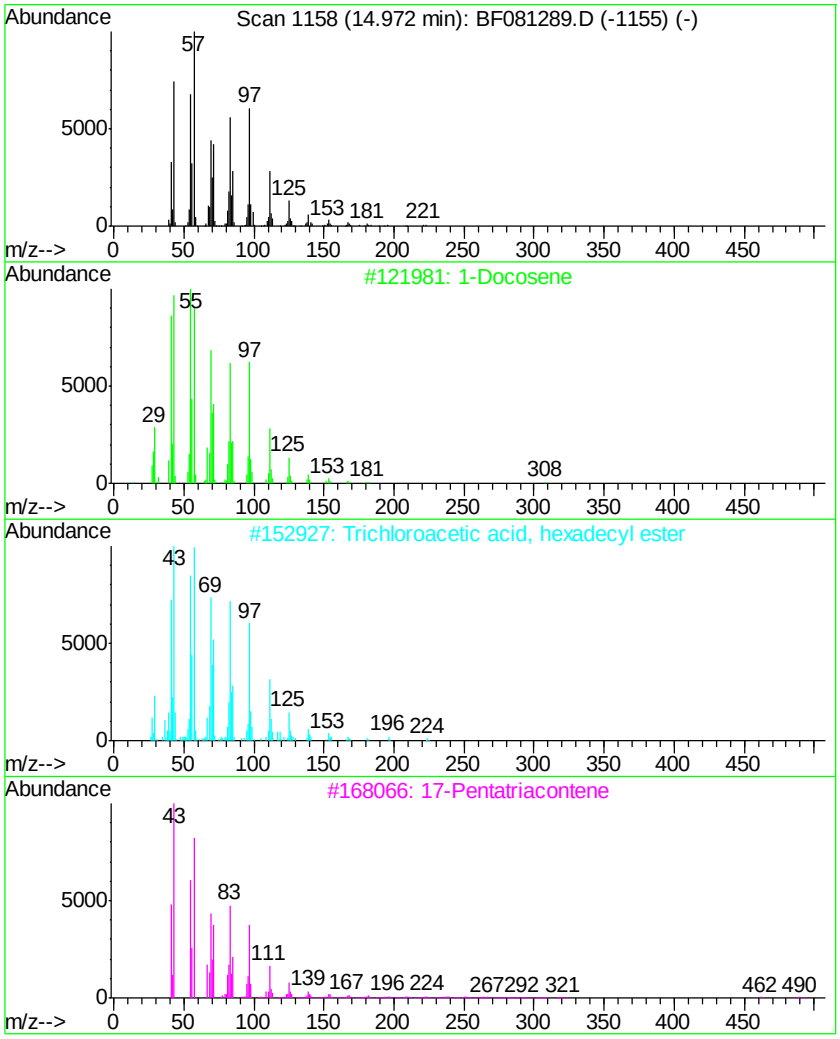
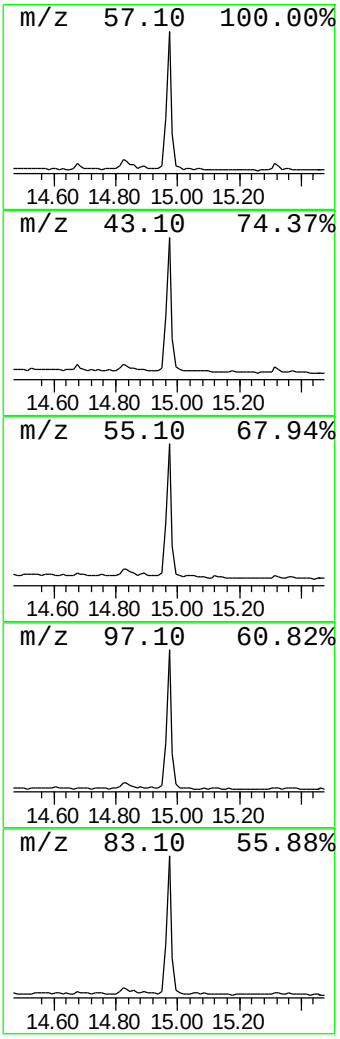
Peak Number 18 1-Docosene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	20.00 ng	427257	Perylene-d12	14.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	87
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
3	17-Pentatriacontene	491	C35H70	006971-40-0	80
4	1-Nonadecene	266	C19H38	018435-45-5	64
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	62





Tentatively Identified Compound (LSC) summary

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Acq On : 30 Aug 2015 00:31
Operator : UM/IZ
Sample : G3467-03
Misc :
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Instrument : BNA_F
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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
Benzene, 1-chloro...	6.00	1668.5	ng	32824300	1	6.48	393466	20.0
Benzene, 1,2,4-tr...	6.54	22.0	ng	432036	1	6.48	393466	20.0
unknown8.16	8.16	23.0	ng	591242	2	7.77	514040	20.0
Phenol, 4-chloro-...	8.21	24.6	ng	631732	2	7.77	514040	20.0
unknown8.25	8.25	19.8	ng	508683	2	7.77	514040	20.0
unknown8.43	8.43	13.5	ng	346955	2	7.77	514040	20.0
Thiazole, 4,5-dih...	8.48	27.0	ng	694548	2	7.77	514040	20.0
Benzoic acid, 4-c...	8.65	24.3	ng	713755	3	9.51	588134	20.0
unknown9.84	9.84	16.2	ng	477267	3	9.51	588134	20.0
unknown9.95	9.95	17.1	ng	503644	3	9.51	588134	20.0
n-Hexadecanoic acid	11.56	13.1	ng	426107	4	10.98	648709	20.0
unknown12.00	12.00	12.7	ng	410502	4	10.98	648709	20.0
2H-1-Benzopyran-2...	12.17	37.4	ng	1213330	4	10.98	648709	20.0
Octadecanoic acid	12.33	30.7	ng	575102	5	13.59	374607	20.0
1-Docosene	14.97	20.0	ng	427257	6	14.92	427257	20.0