LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077930.D
Acq On : 25 Mar 2015 2:12
Operator : TP/IZ
Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

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-BF031115.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	1.264	31	33	36	rVB	2760214	2804717	100.00%	22.809%
2	1.390	41	44	56	rVB	73778	164650	5.87%	1.339%
3	1.550	56	58	65	rVB	42040	52537	1.87%	0.427%
4	1.653	65	67	75	rVB	53405	83889	2.99%	0.682%
5	1.767	75	77	106	rVB	550673	1044823	37.25%	8.497%
6	4.864	345	348	354	rBV	58342	75871	2.71%	0.617%
7	5.401	392	395	403	rBV	505737	630471	22.48%	5.127%
8	6.693	505	508	510	rBV	538797	653573	23.30%	5.315%
9	6.830	517	520	522	rBV	624133	703437	25.08%	5.721%
10	7.116	543	545	547	rBV	258831	237415	8.46%	1.931%
11	7.299	559	561	564	rBV	617073	557845	19.89%	4.537%
12	7.813	603	606	608	rBV	356692	395290	14.09%	3.215%
13	8.693	681	683	685	rBV	354774	327946	11.69%	2.667%
14	10.042	798	801	803	rBV	951931	947920	33.80%	7.709%
15	10.545	843	845	848	rBV	41963	40332	1.44%	0.328%
16	10.865	870	873	875	rBV	303027	376864	13.44%	3.065%
17	11.768	949	952	954	rBV	76920	102534	3.66%	0.834%
18	11.836	956	958	961	rBV	501631	483074	17.22%	3.929%
19	12.694	1031	1033	1036	rBV	427311	414364	14.77%	3.370%
20	14.694	1205	1208	1210	rBV	1003695	1165866	41.57%	9.481%
21	15.974	1318	1320	1323	rBV	466453	474719	16.93%	3.861%
22	17.711	1470	1472	1475	rBV	323370	454380	16.20%	3.695%
23	19.083	1586	1592	1601	rVB	24565	103917	3.71%	0.845%

Sum of corrected areas: 12296434

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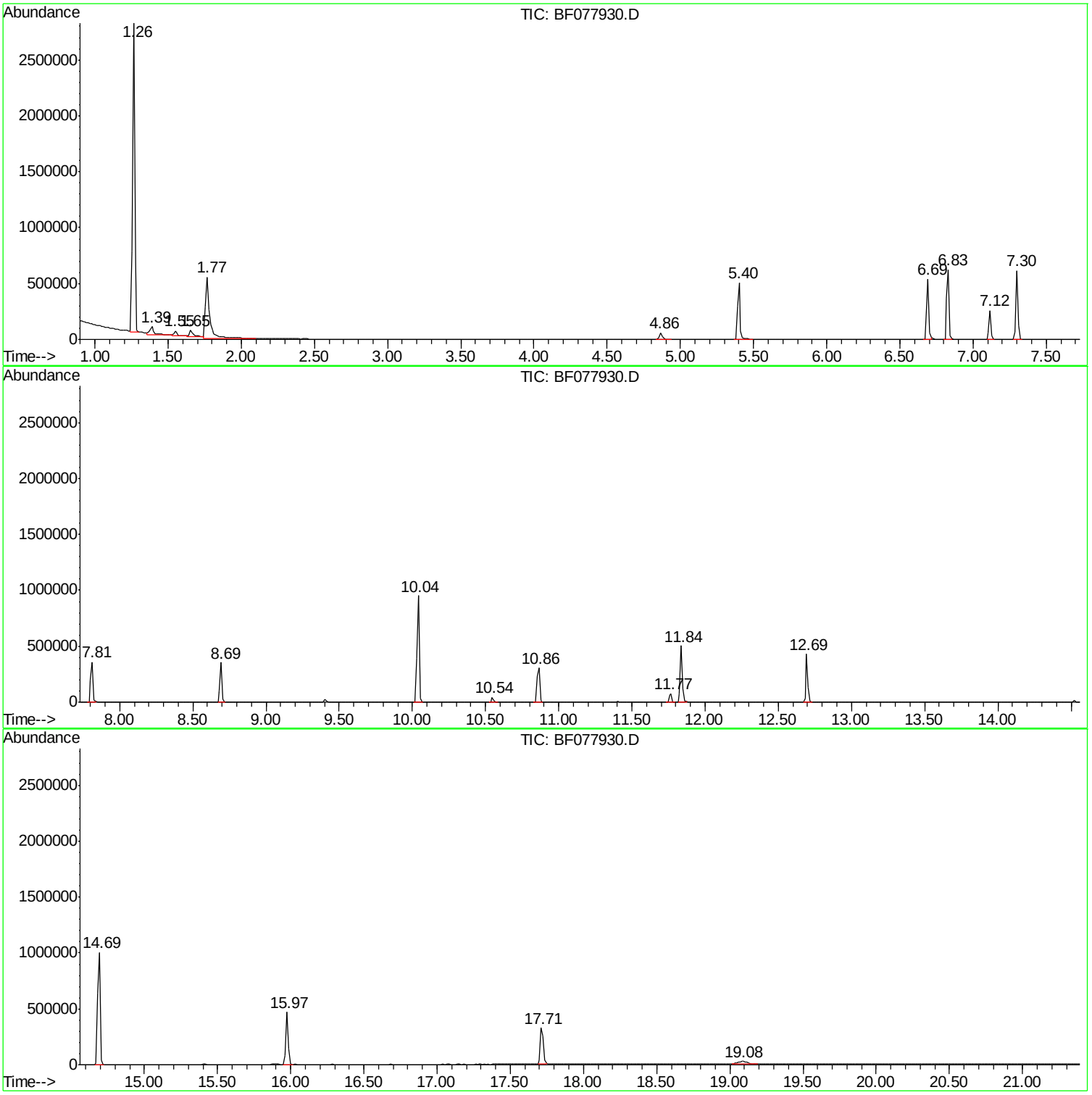
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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\BF032415\
Data File : BF077930.D
Acq On : 25 Mar 2015 2:12
Operator : TP/IZ
Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

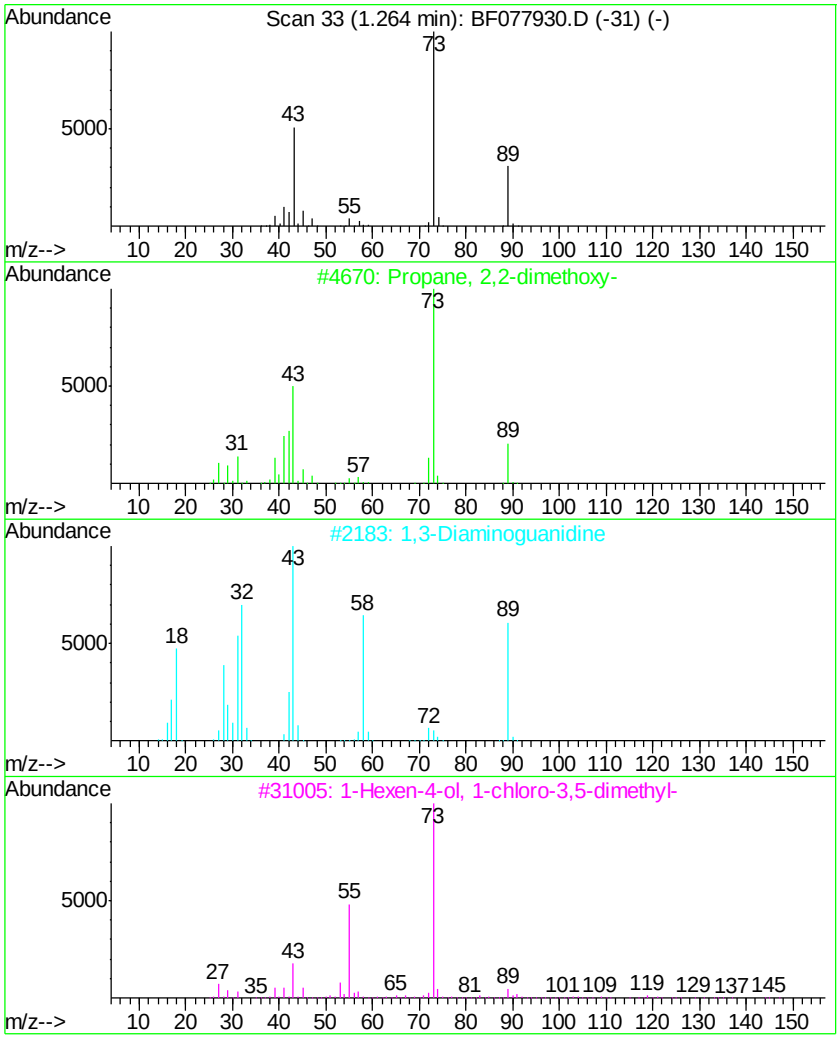
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

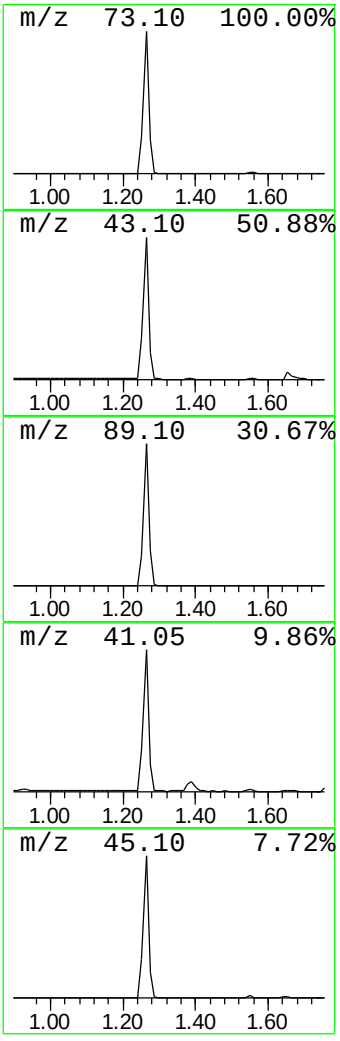
****

Peak Number 1 unknown1.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	236.27 ng	2804720	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077930.D
Acq On : 25 Mar 2015 2:12
Operator : TP/IZ
Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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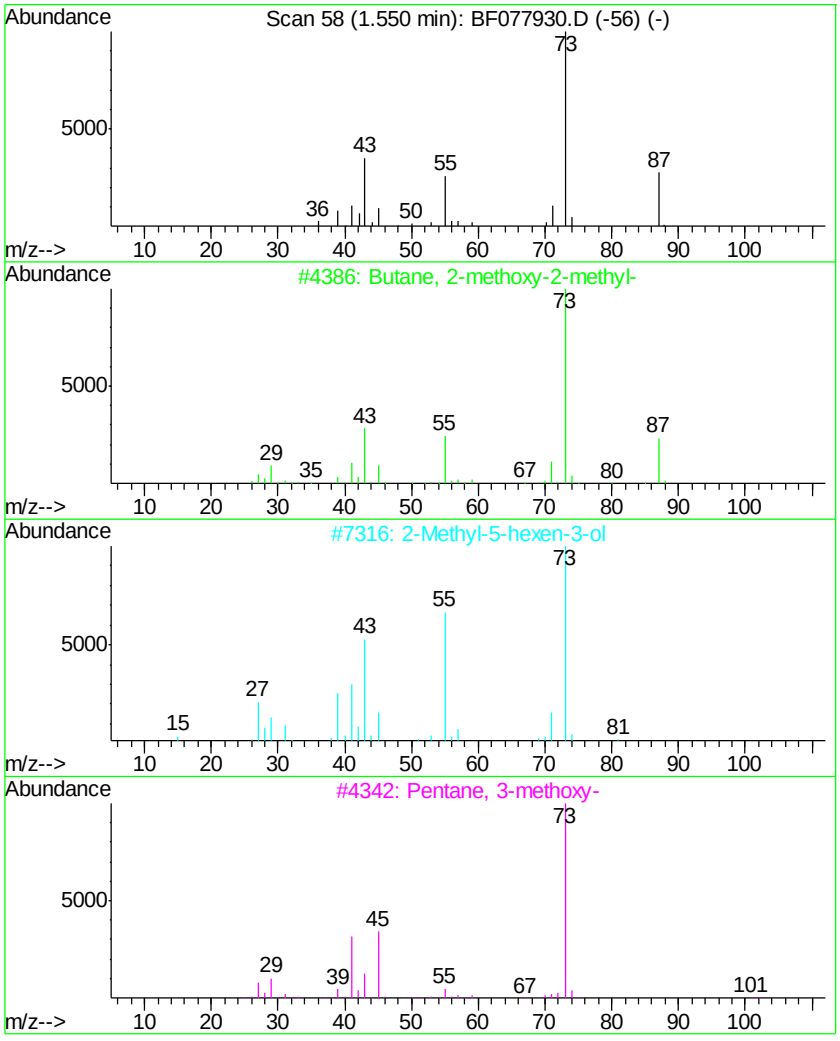
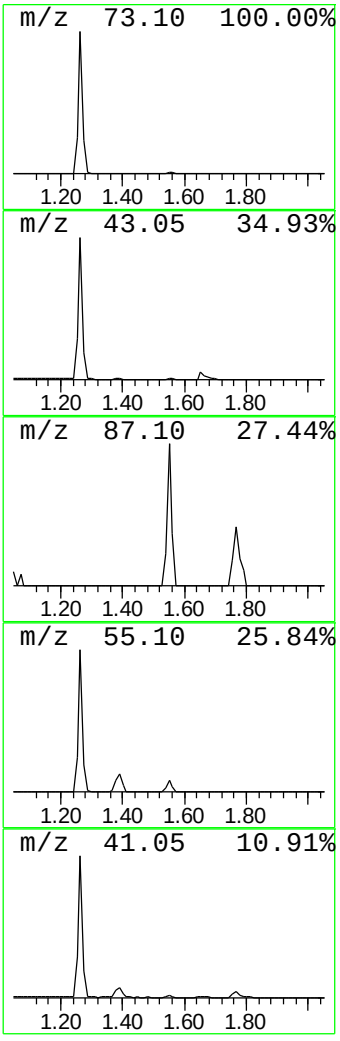
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	4.43 ng	52537	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077930.D
Acq On : 25 Mar 2015 2:12
Operator : TP/IZ
Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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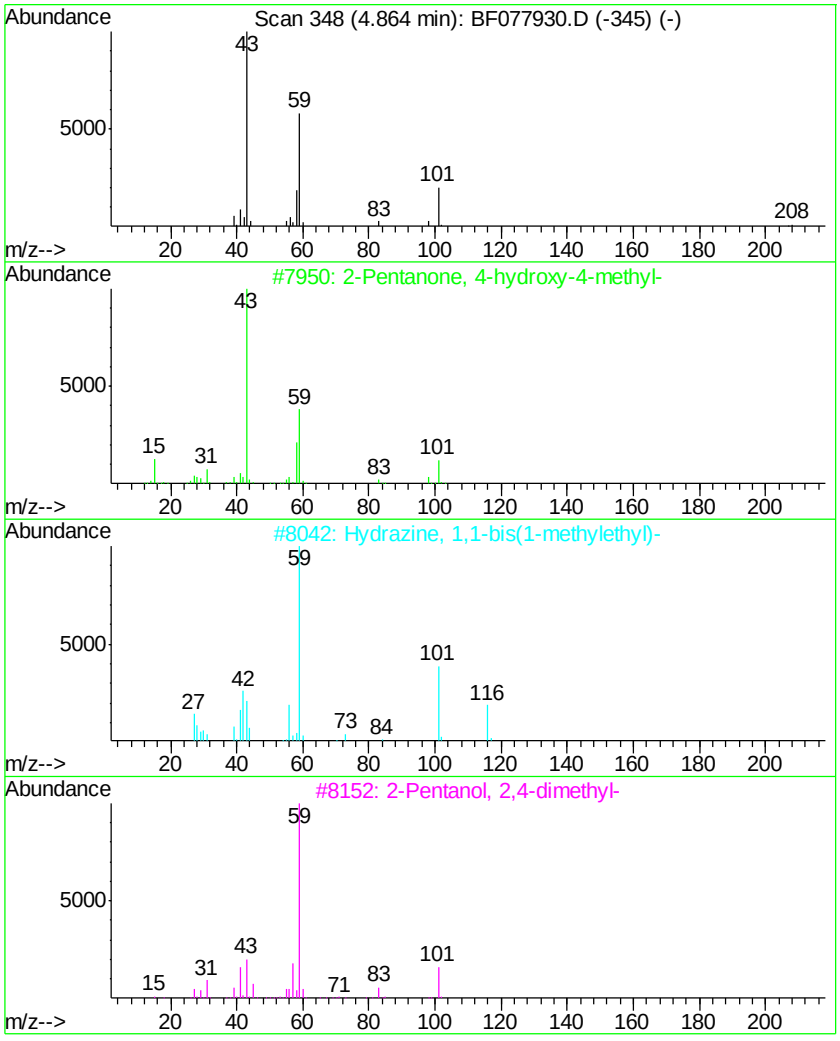
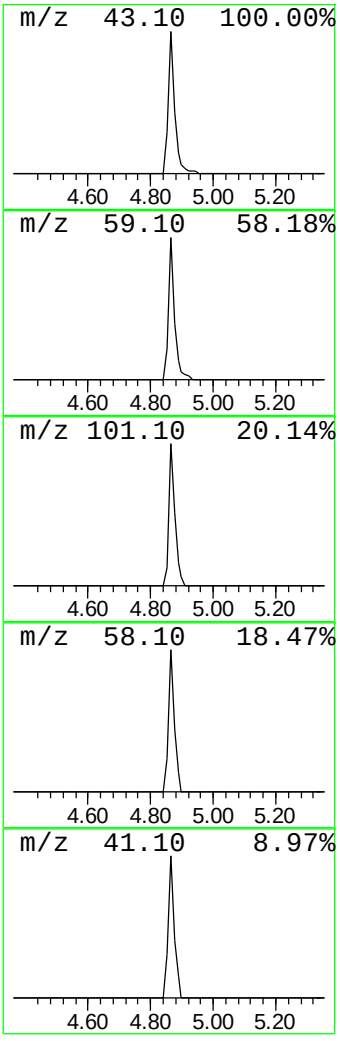
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	6.39 ng	75871	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BF077930.D
Acq On : 25 Mar 2015 2:12
Operator : TP/IZ
Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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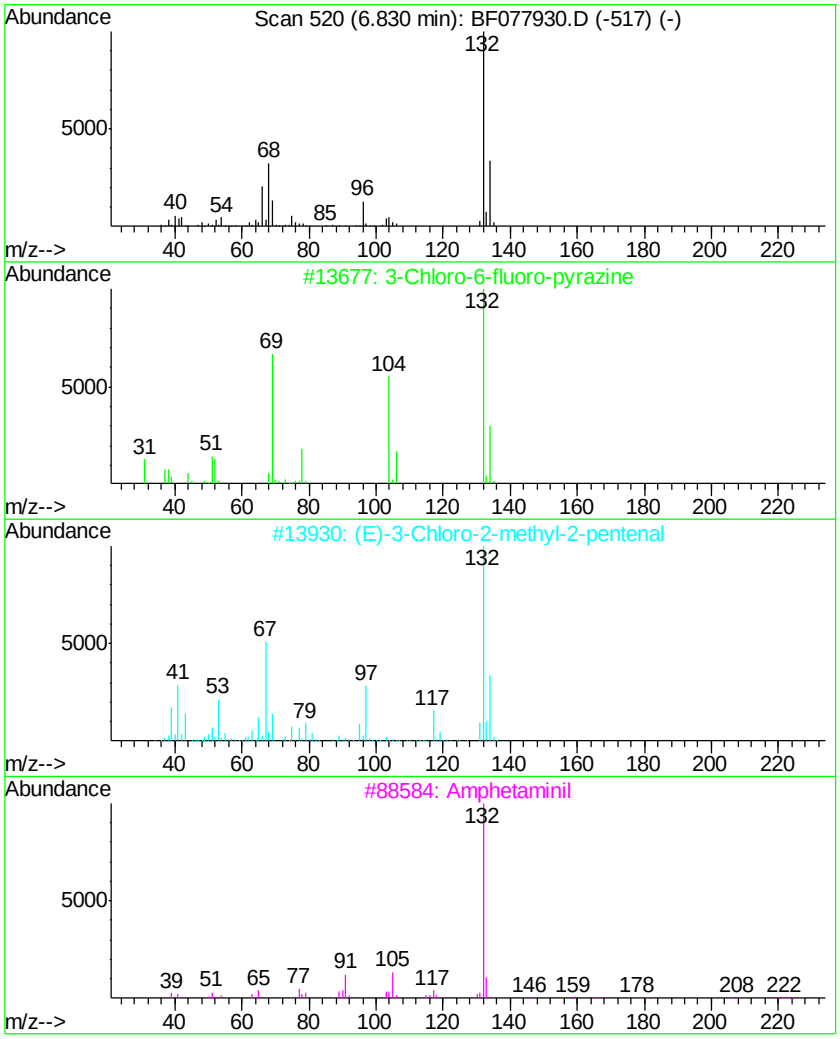
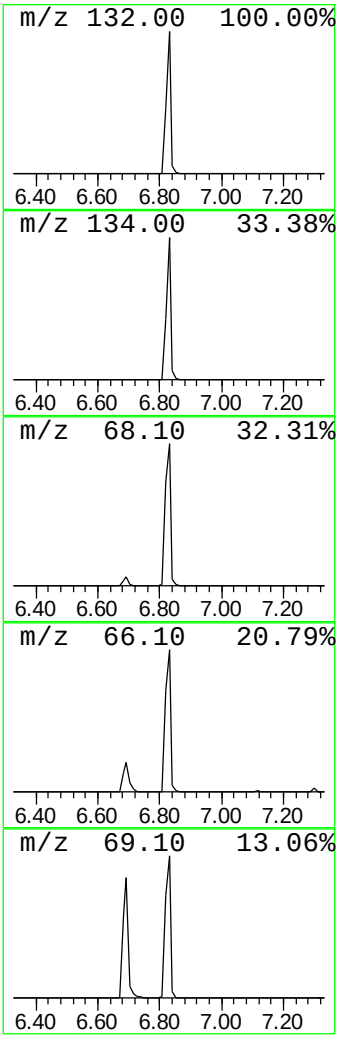
Peak Number 7 unknown6.83 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	59.26 ng	703437	1,4-Dichlorobenzene-d4	7.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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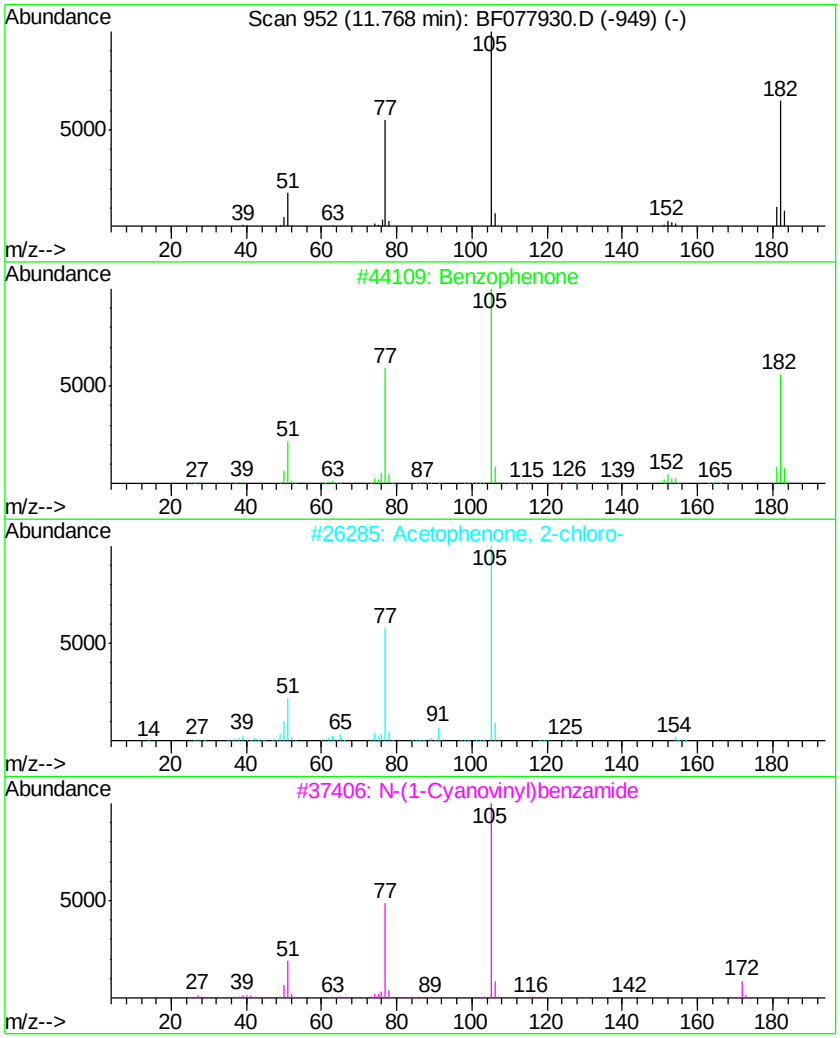
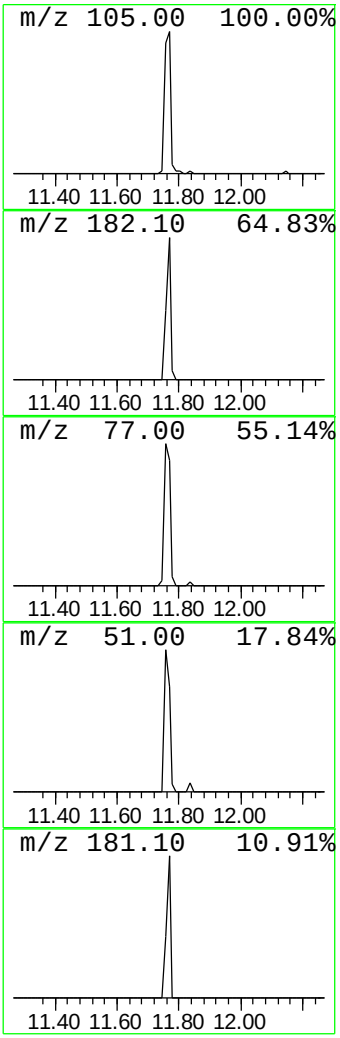
Peak Number 9 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.44 ng	102534	Acenaphthene-d10	10.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
3	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	43
4	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	43
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43





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Sample : G1613-19
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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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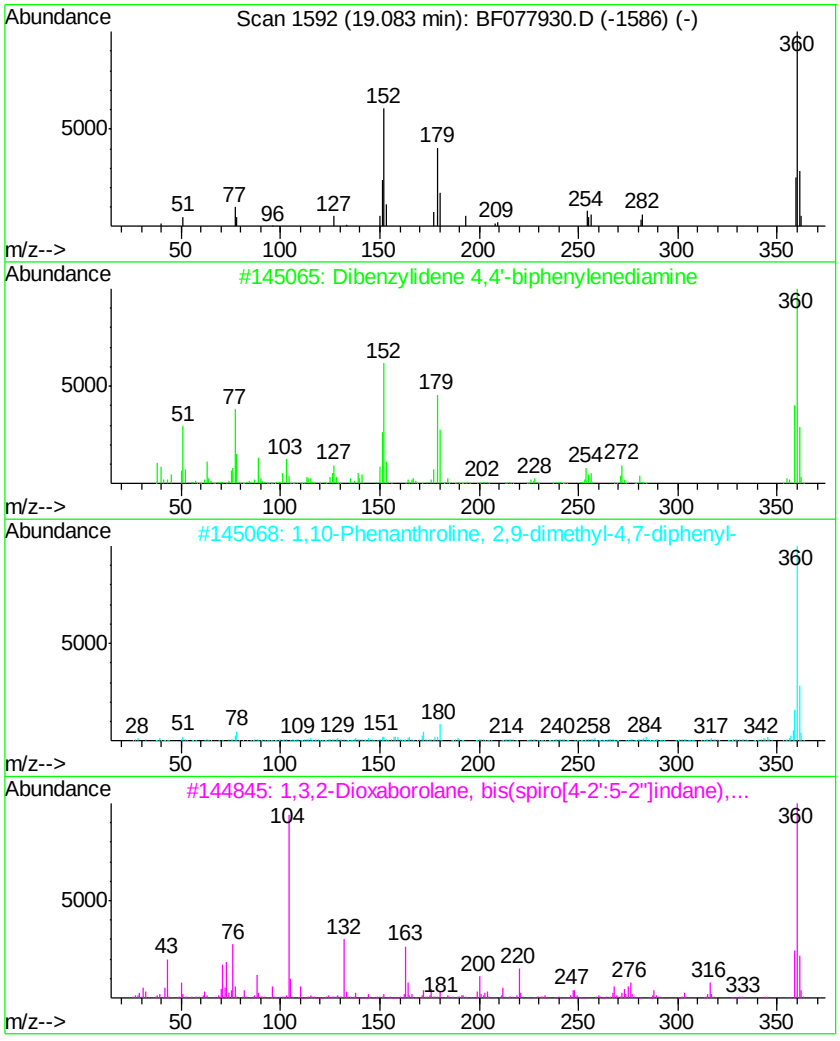
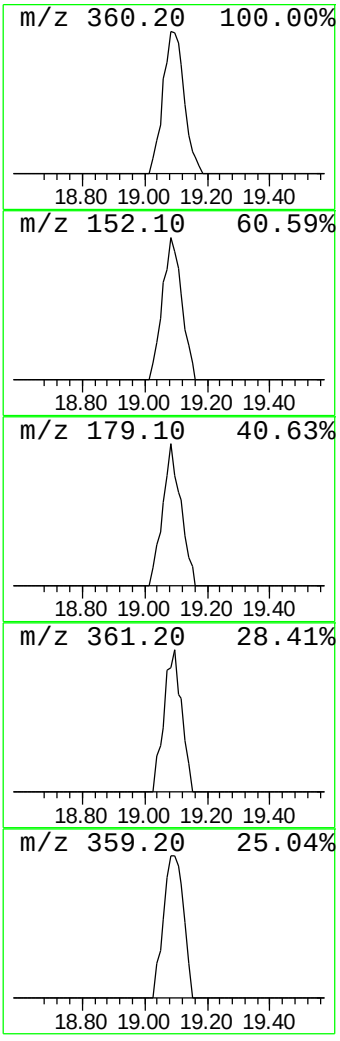
Peak Number 10 Dibenzylidene 4,4'-biphenyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.08	4.57 ng	103917	Perylene-d12	17.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	38
3	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	38
4	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	38
5	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
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ClientSampleId : SB-13

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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
unknown1.26	1.26	236.3	ng	2804720	1	7.12	237415	20.0
Butane, 2-methoxy...	1.55	4.4	ng	52537	1	7.12	237415	20.0
2-Pentanone, 4-hy...	4.86	6.4	ng	75871	1	7.12	237415	20.0
unknown6.83	6.83	59.3	ng	703437	1	7.12	237415	20.0
Benzophenone	11.77	5.4	ng	102534	3	10.86	376864	20.0
Dibenzylidene 4,4...	19.08	4.6	ng	103917	6	17.71	454380	20.0