LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088073.D
Acq On : 16 Jun 2016 13:58
Operator : UM/SJ
Sample : H3510-01RE
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

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-BF060716.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	1.804	17	19	22	rBV	635927	1267443	41.74%	5.035%
2	2.467	76	77	82	rVB	52630	82366	2.71%	0.327%
3	3.176	136	139	147	rBV	188848	339138	11.17%	1.347%
4	4.227	227	231	234	rBV	1672367	3036674	100.00%	12.064%
5	4.524	254	257	259	rBV	56253	85930	2.83%	0.341%
6	4.913	288	291	299	rBV	74071	118950	3.92%	0.473%
7	5.164	311	313	317	rVB	22018	34071	1.12%	0.135%
8	5.324	324	327	329	rBV	1956325	2096875	69.05%	8.330%
9	6.365	415	418	420	rBV	1574984	1583461	52.14%	6.291%
10	6.490	426	429	431	rBV	2250442	2184493	71.94%	8.679%
11	6.719	447	449	451	rBV	684433	564181	18.58%	2.241%
12	6.879	460	463	465	rVB	1626036	1915336	63.07%	7.609%
13	6.936	466	468	470	rVB	68499	54063	1.78%	0.215%
14	7.016	473	475	478	rVB2	186156	226263	7.45%	0.899%
15	7.290	496	499	501	rBV	1426479	1671821	55.05%	6.642%
16	7.999	559	561	567	rBB	767446	817751	26.93%	3.249%
17	8.525	605	607	611	rBV2	41232	44729	1.47%	0.178%
18	8.799	630	631	634	rVB	110944	107493	3.54%	0.427%
19	9.085	652	656	658	rBV	2574351	2919687	96.15%	11.599%
20	9.748	712	714	716	rBV	457346	495945	16.33%	1.970%
21	10.536	780	783	786	rBV	1363999	1572220	51.77%	6.246%
22	11.234	841	844	846	rBV	747235	783872	25.81%	3.114%
23	12.822	980	983	985	rBV	2100935	2608389	85.90%	10.363%
24	13.862	1071	1074	1080	rVB	344643	394685	13.00%	1.568%
25	15.268	1193	1197	1200	rBV3	41508	80303	2.64%	0.319%
26	15.394	1203	1208	1216	rBV2	22805	85064	2.80%	0.338%

Sum of corrected areas: 25171203

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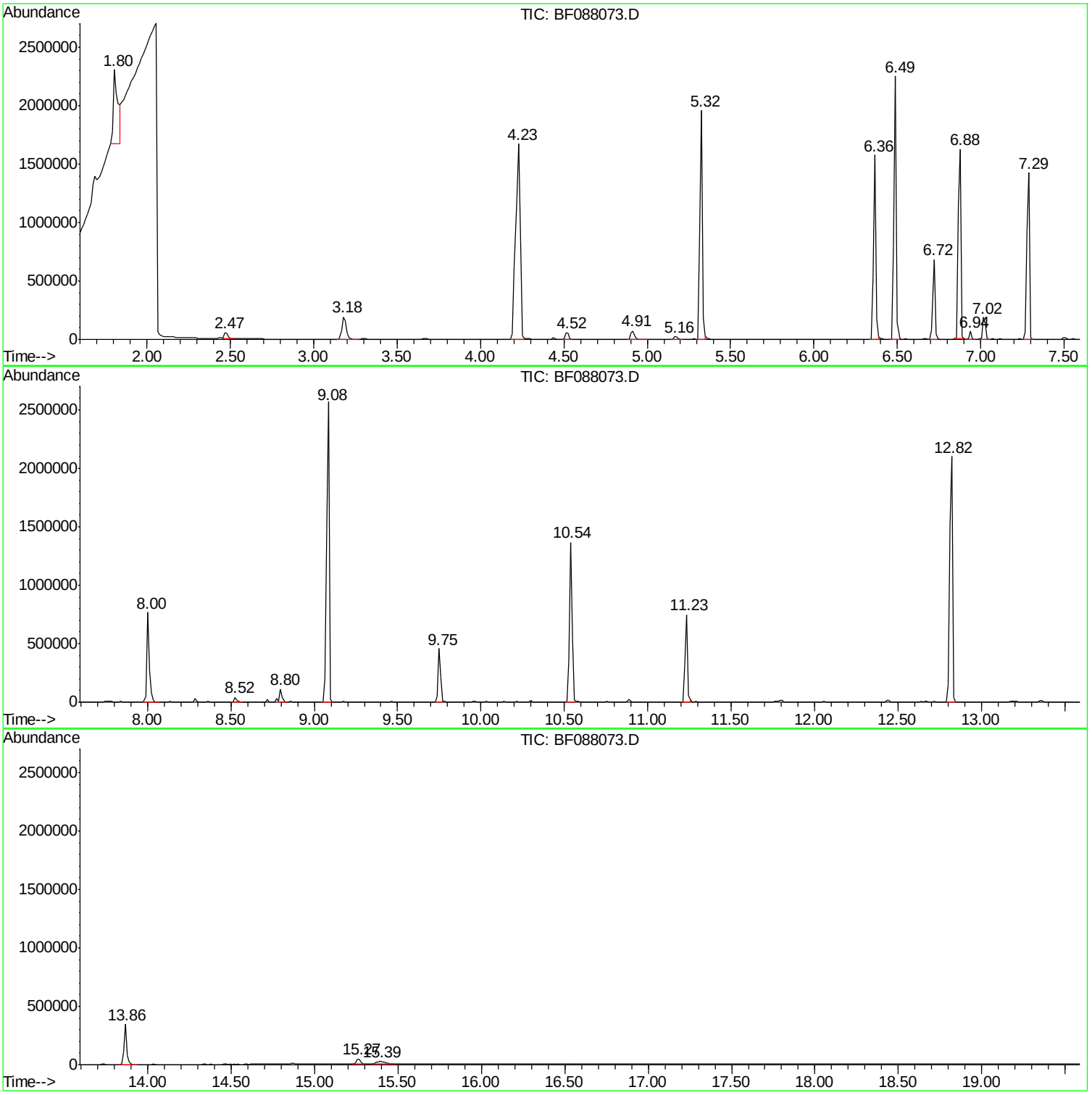
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF088073.D
Acq On : 16 Jun 2016 13:58
Operator : UM/SJ
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Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

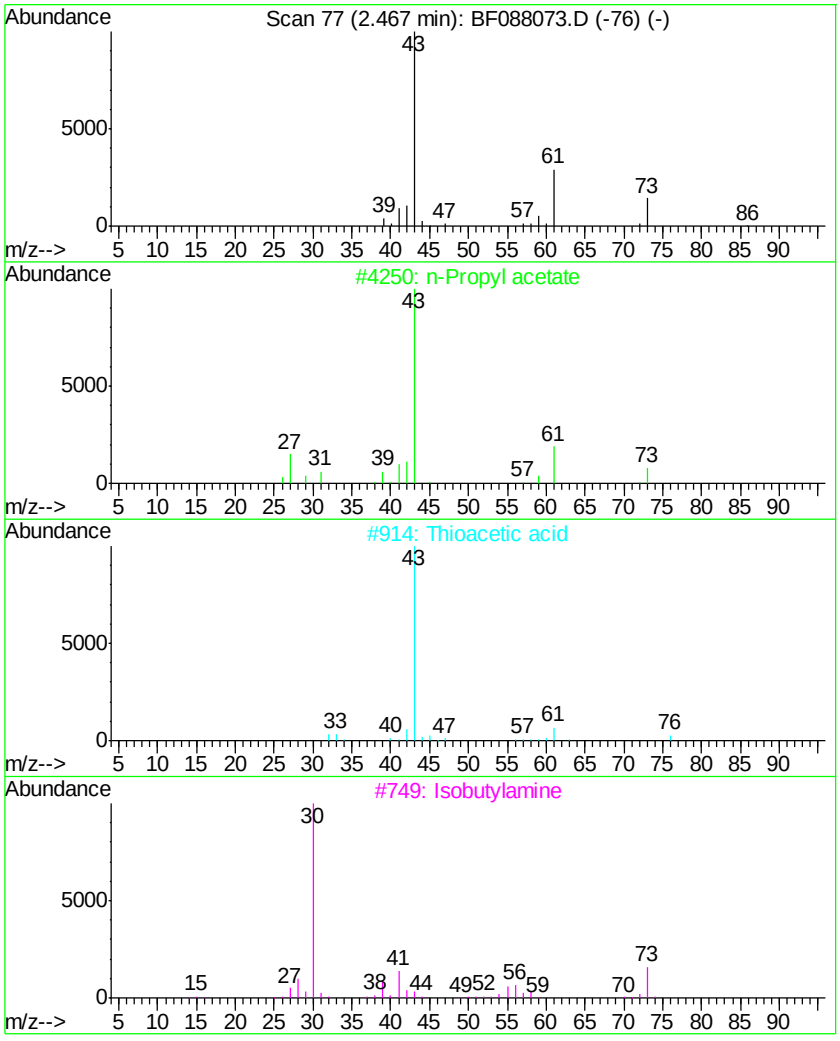
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

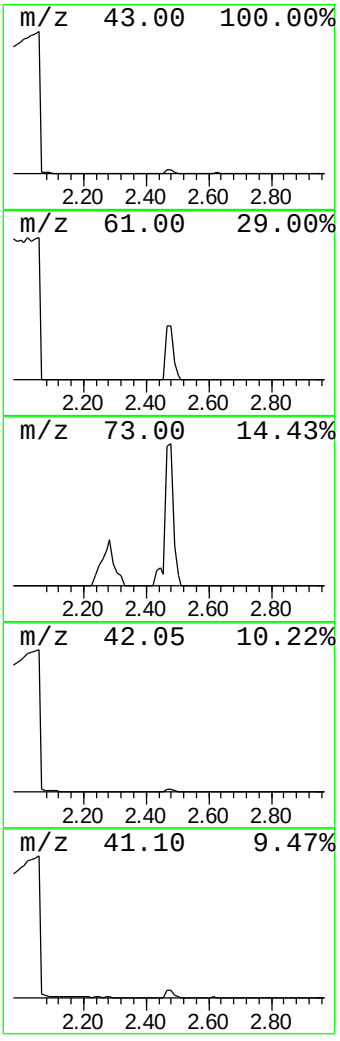
****

Peak Number 2 n-Propyl acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.47	2.92 ng	82366	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Thioacetic acid	76	C2H4OS	000507-09-5	25
3	Isobutylamine	73	C4H11N	000078-81-9	7
4	1-Butanamine	73	C4H11N	000109-73-9	5
5	Isobutane	58	C4H10	000075-28-5	5





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Data File : BF088073.D
Acq On : 16 Jun 2016 13:58
Operator : UM/SJ
Sample : H3510-01RE
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

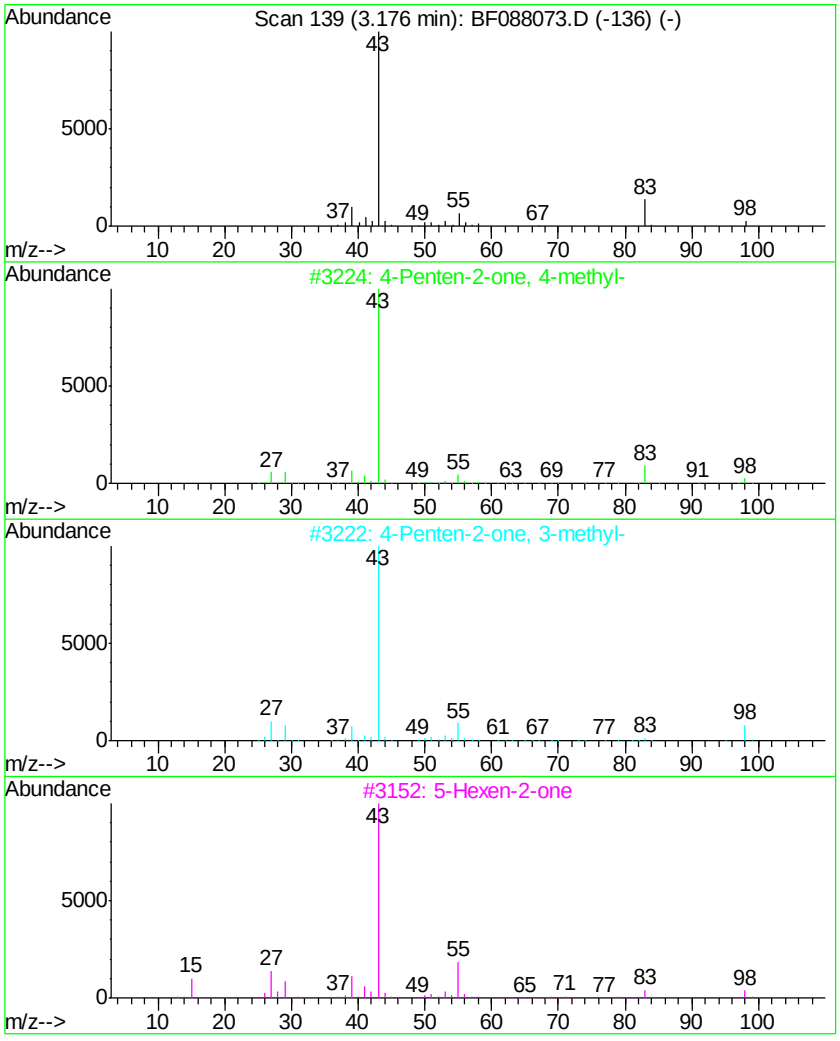
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

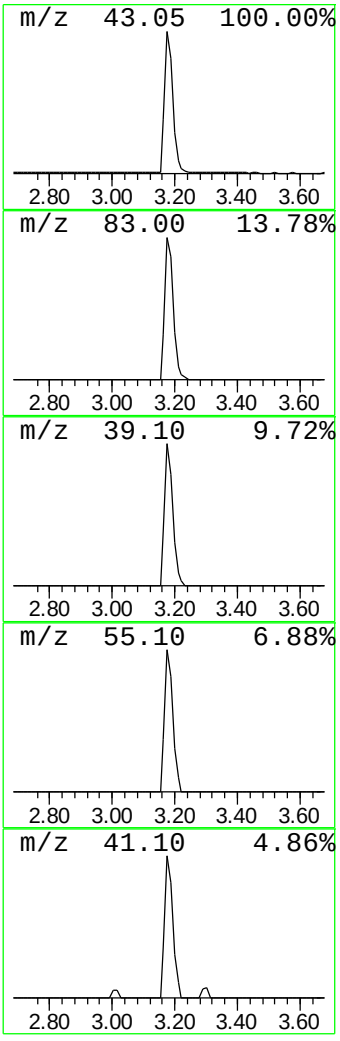
****

Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	12.02 ng	339138	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3	5-Hexen-2-one	98	C6H10O	000109-49-9	50
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088073.D
Acq On : 16 Jun 2016 13:58
Operator : UM/SJ
Sample : H3510-01RE
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

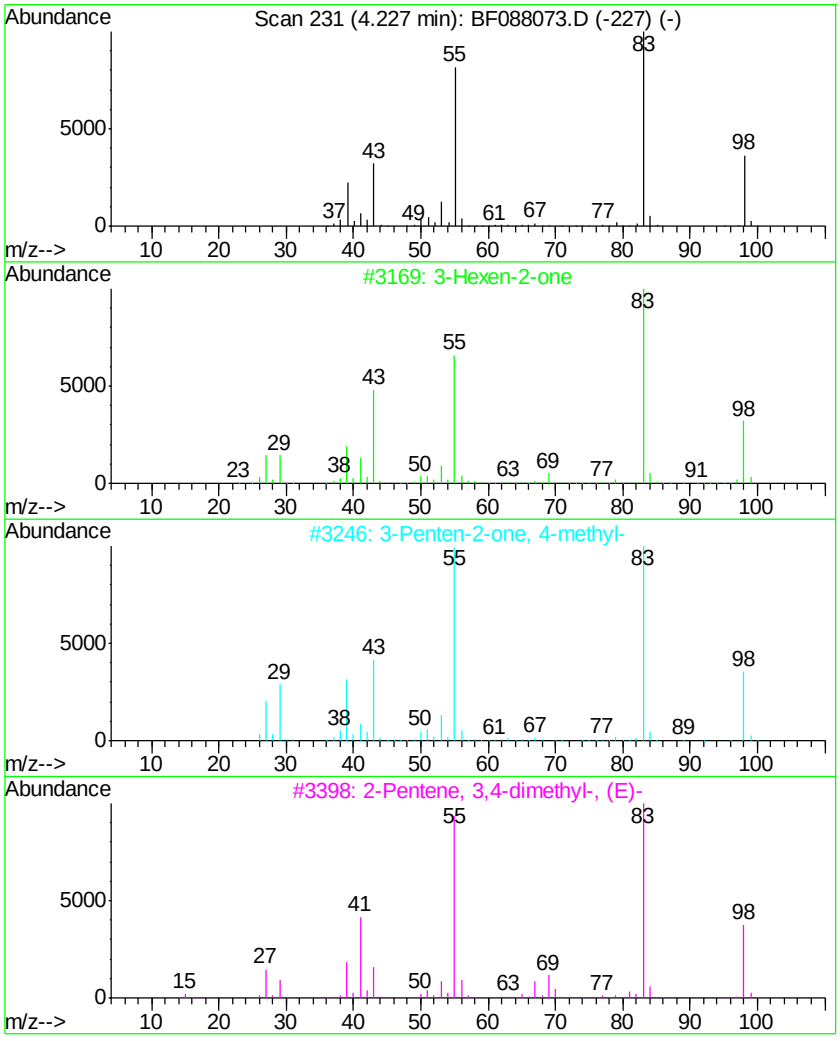
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

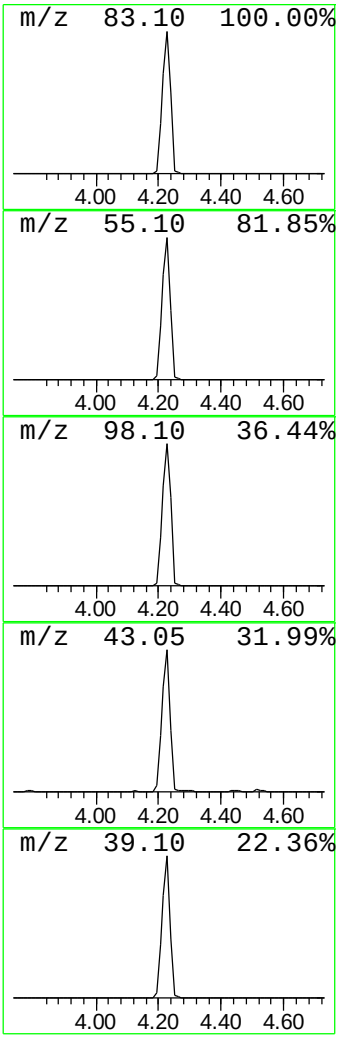
****

Peak Number 4 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.23	107.65 ng	3036670	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Sample : H3510-01RE
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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

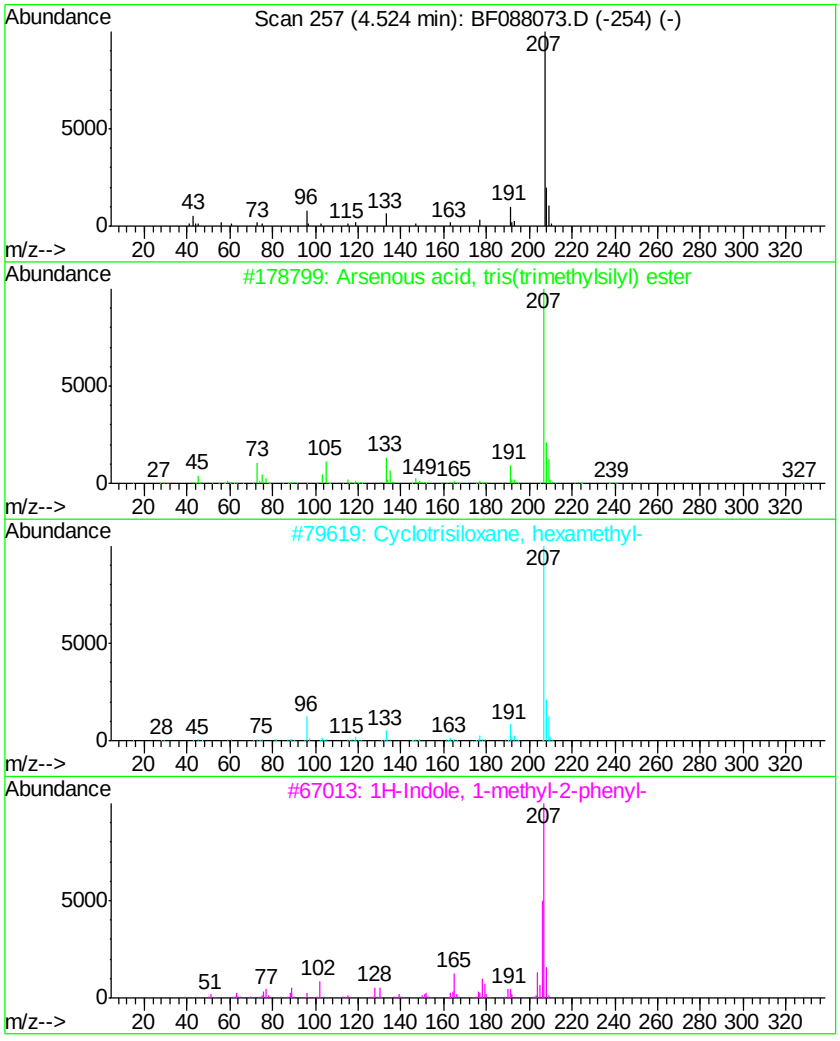
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

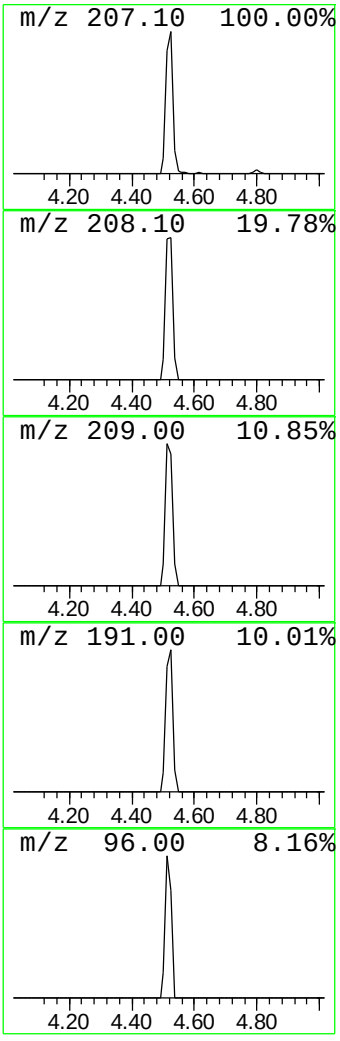
****

Peak Number 5 Arsenous acid, tris(trimeth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	3.05 ng	85930	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	74
2	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	53
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	50
4	2-Ethylacridine	207	C15H13N	055751-83-2	45
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39





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Operator : UM/SJ
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

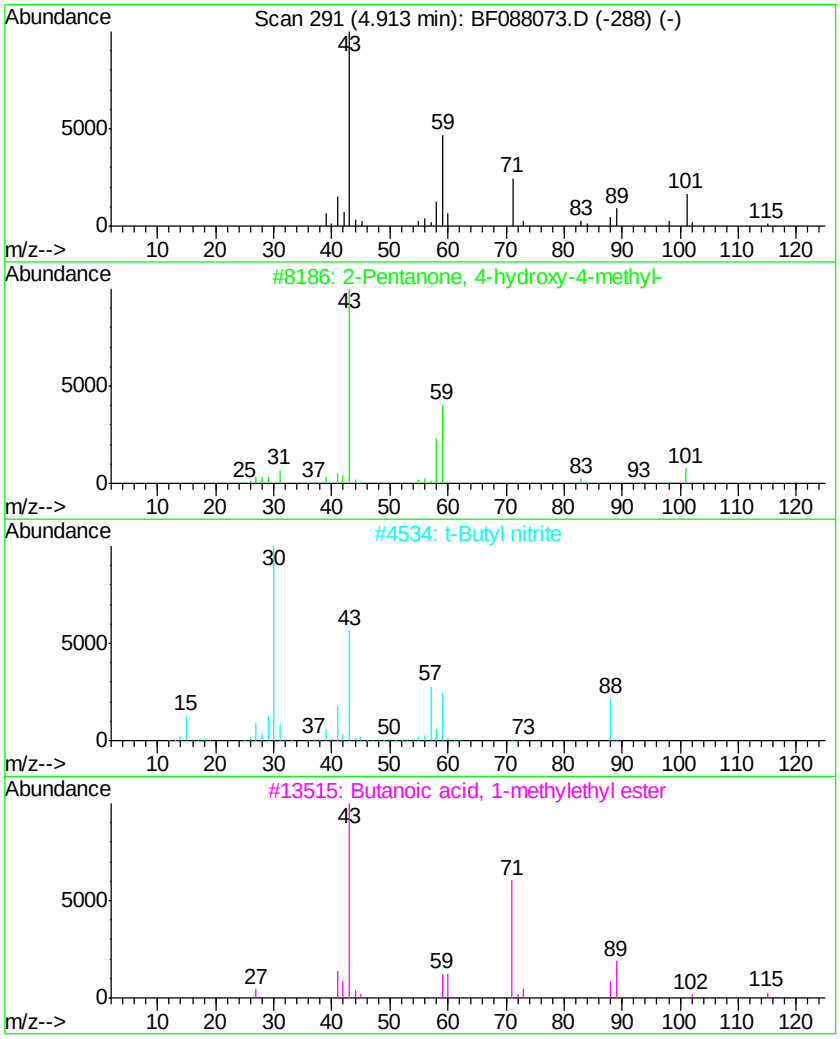
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

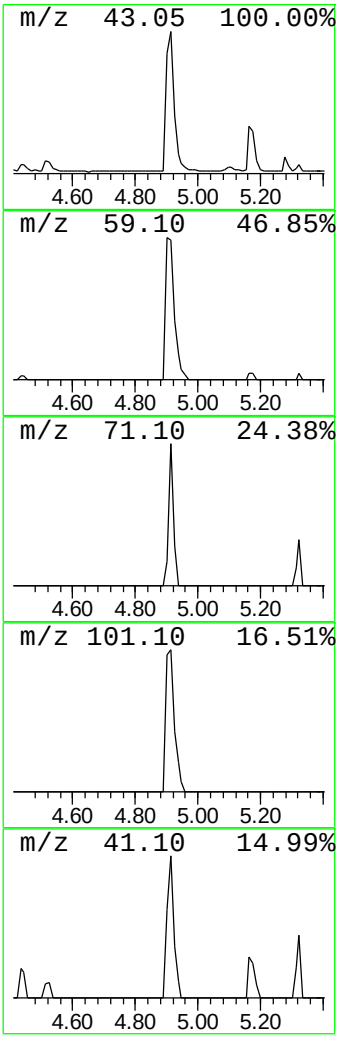
****

Peak Number 6 unknown4.91 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.22 ng	118950	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	28
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	12
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : H3510-01RE
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

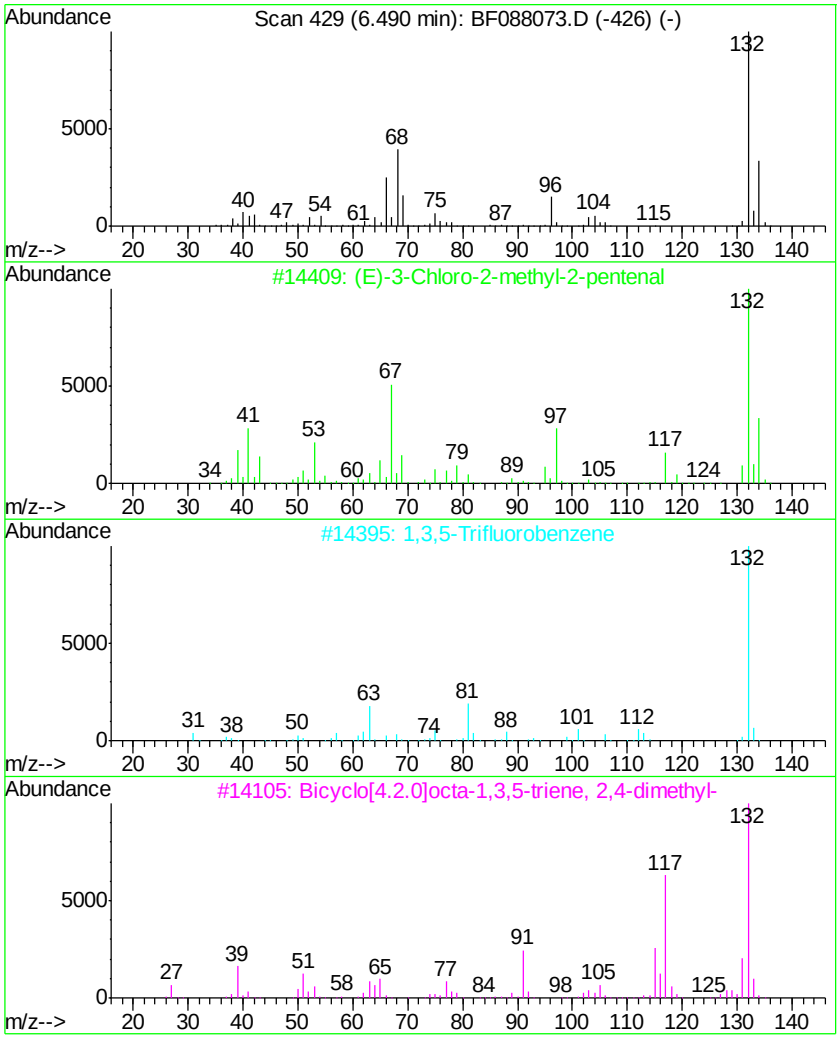
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

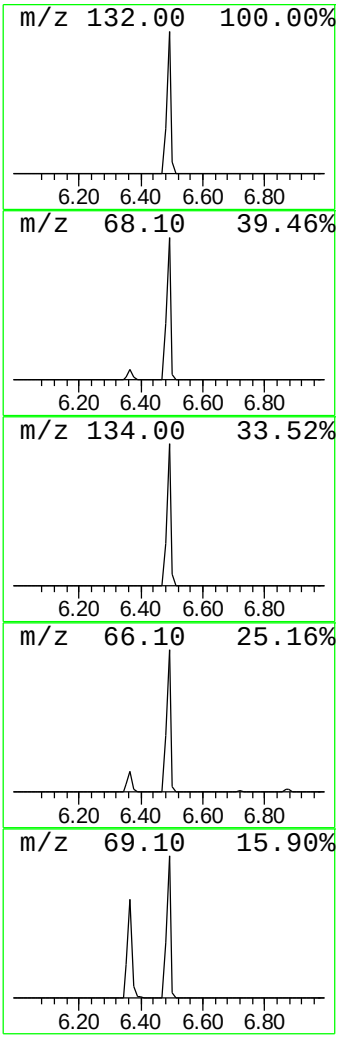
****

Peak Number 7 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	77.44 ng	2184490	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : H3510-01RE
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Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

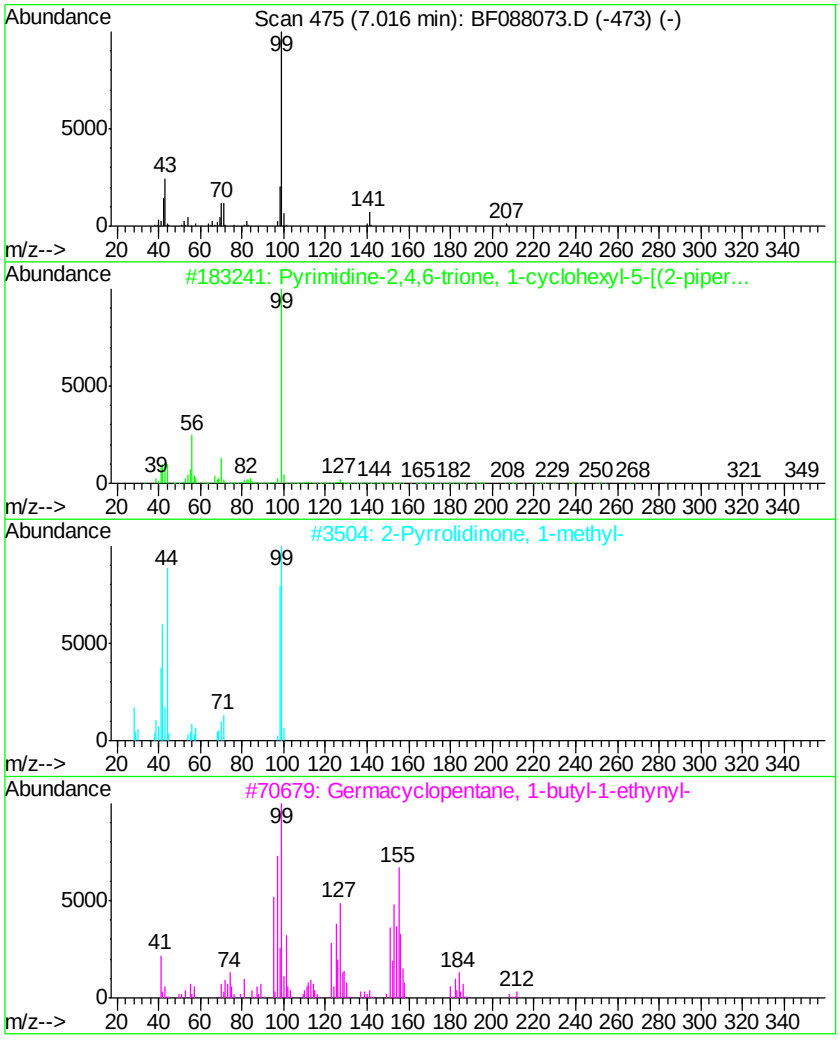
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

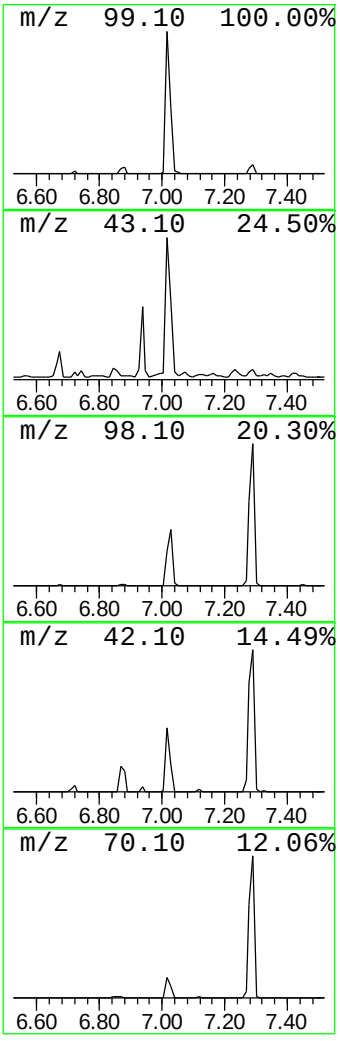
****

Peak Number 9 Pyrimidine-2,4,6-trione, 1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	8.02 ng	226263	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidine-2,4,6-trione, 1-cyclo...	349	C17H27N5O3	1000304-66-3	59
2	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	53
3	Germacyclopentane, 1-butyl-1-eth...	212	C10H18Ge	004554-80-7	50
4	2-Piperidinone	99	C5H9NO	000675-20-7	45
5	Octadecane, 1-isocyanato-	295	C19H37NO	000112-96-9	40





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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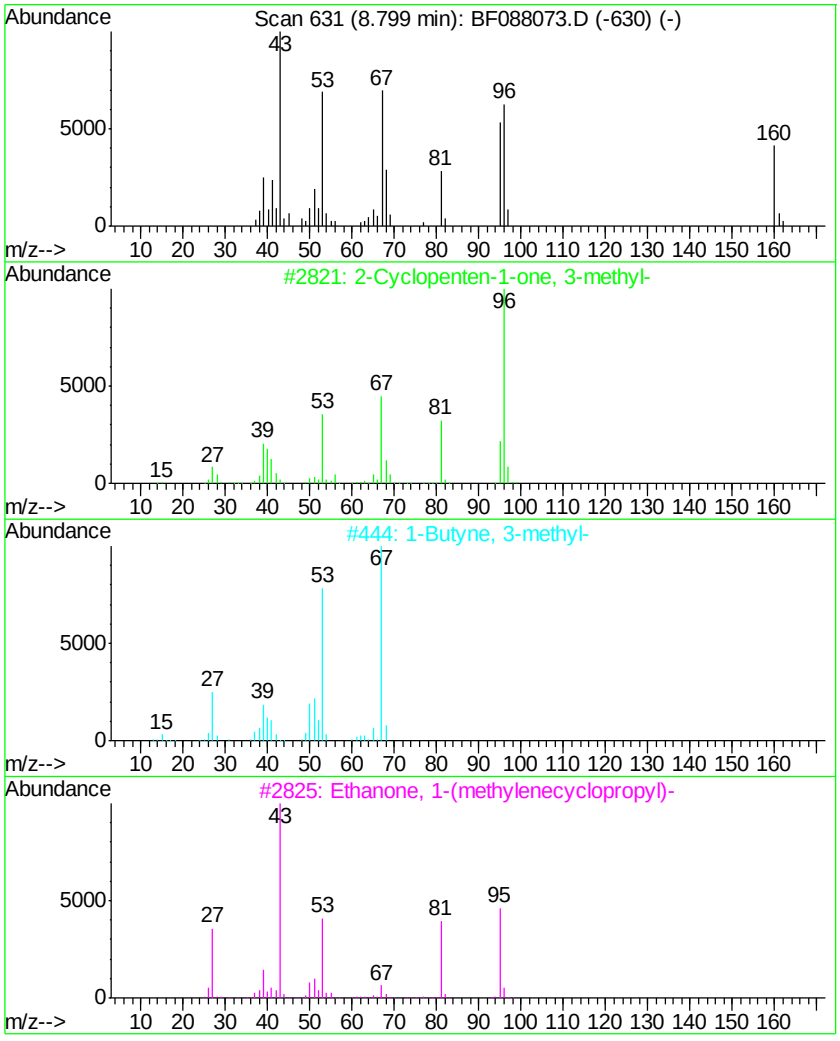
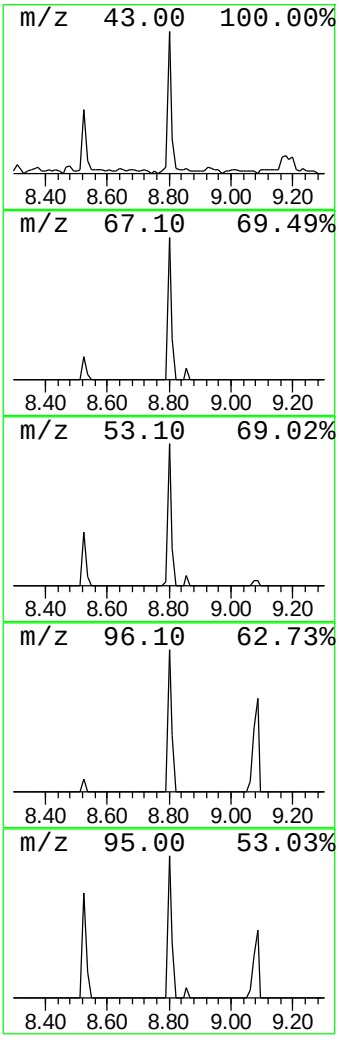
****

Peak Number 10 2-Cyclopenten-1-one, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.63 ng	107493	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	76
2	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	43
3	Ethanone, 1-(methylenecyclopropyl)-	96	C6H8O	062266-35-7	43
4	1,2,4-Triazine	81	C3H3N3	000290-38-0	35
5	2,4-Dimethylfuran	96	C6H8O	003710-43-8	30





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Instrument : BNA_F
ClientSampleId : HSR-WC-52-060916RE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

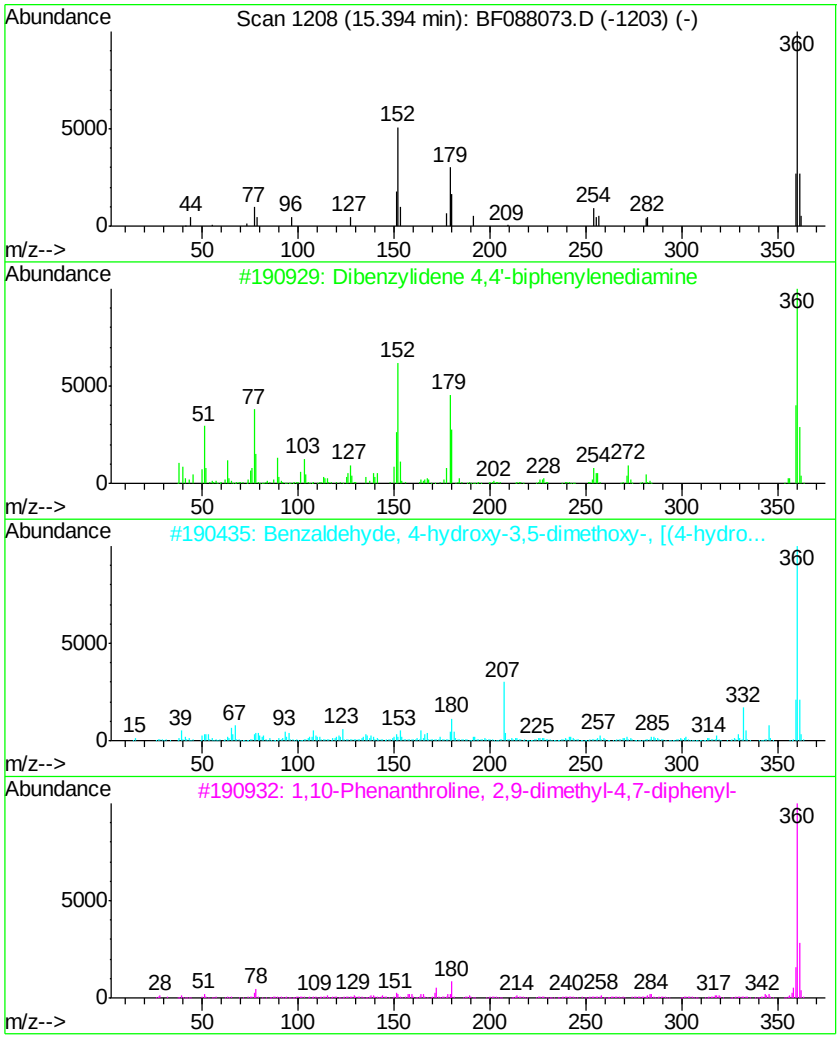
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

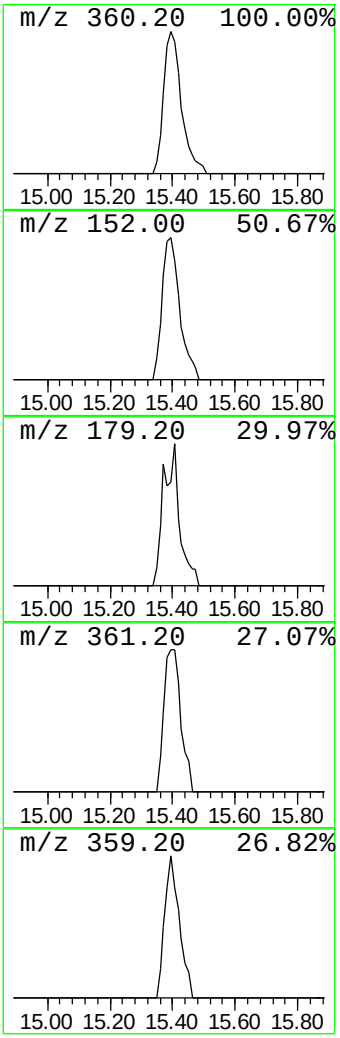
****

Peak Number 11 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	21.19 ng	85064	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	95
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
3	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
4	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	43
5	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
Data File : BF088073.D
Acq On : 16 Jun 2016 13:58
Operator : UM/SJ
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Misc :
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Instrument : BNA_F
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TIC Library : C:\Database\NIST11.L
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.47	2.9	ng	82366	1	6.72	564181	20.0
4-Penten-2-one, 4...	3.18	12.0	ng	339138	1	6.72	564181	20.0
3-Hexen-2-one	4.23	107.7	ng	3036670	1	6.72	564181	20.0
Arsenous acid, tr...	4.52	3.0	ng	85930	1	6.72	564181	20.0
unknown4.91	4.91	4.2	ng	118950	1	6.72	564181	20.0
unknown6.49	6.49	77.4	ng	2184490	1	6.72	564181	20.0
Pyrimidine-2,4,6-...	7.02	8.0	ng	226263	1	6.72	564181	20.0
2-Cyclopenten-1-o...	8.80	2.6	ng	107493	2	8.00	817751	20.0
Dibenzylidene 4,4...	15.39	21.2	ng	85064	6	15.26	80303	20.0