LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF022218\
Data File : BF103168.D
Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

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-BF022218.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	2.146	5	10	26	rVB	869319	1270159	8.90%	2.897%
2	3.604	252	258	270	rBV	333397	526146	3.69%	1.200%
3	4.516	401	413	416	rBV	5462027	14263614	100.00%	32.533%
4	5.134	507	518	521	rBV	4198299	9731098	68.22%	22.195%
5	5.710	612	616	620	rBV	172614	147394	1.03%	0.336%
6	6.498	745	750	761	rBV2	683269	714748	5.01%	1.630%
7	6.869	810	813	817	rBV	1117203	946714	6.64%	2.159%
8	7.028	836	840	843	rBV	2572833	2265240	15.88%	5.167%
9	7.192	865	868	877	rBV	224888	192518	1.35%	0.439%
10	7.434	904	909	912	rBV	1987927	1791282	12.56%	4.086%
11	8.151	1028	1031	1035	rBV	1249365	1194377	8.37%	2.724%
12	9.228	1210	1214	1217	rBV	3239693	2830711	19.85%	6.456%
13	9.622	1275	1281	1288	rBV	226726	235828	1.65%	0.538%
14	9.910	1326	1330	1334	rBV	1315687	1133159	7.94%	2.585%
15	10.328	1394	1401	1404	rBV2	163593	189327	1.33%	0.432%
16	11.169	1541	1544	1549	rVB	252600	203062	1.42%	0.463%
17	11.398	1580	1583	1587	rBV	896497	848208	5.95%	1.935%
18	12.980	1848	1852	1856	rBV	1810961	1788437	12.54%	4.079%
19	13.839	1995	1998	2001	rBV	496771	413759	2.90%	0.944%
20	14.045	2029	2033	2040	rVB	807933	815908	5.72%	1.861%
21	14.168	2051	2054	2058	rBV	443714	382856	2.68%	0.873%
22	14.210	2058	2061	2063	rVV	697390	565840	3.97%	1.291%
23	14.239	2063	2066	2068	rVV	193376	193286	1.36%	0.441%
24	14.263	2068	2070	2073	rVB	236141	180983	1.27%	0.413%
25	14.886	2173	2176	2187	rVB4	202061	385047	2.70%	0.878%
26	15.539	2283	2287	2293	rVB	503196	634323	4.45%	1.447%

Sum of corrected areas: 43844024

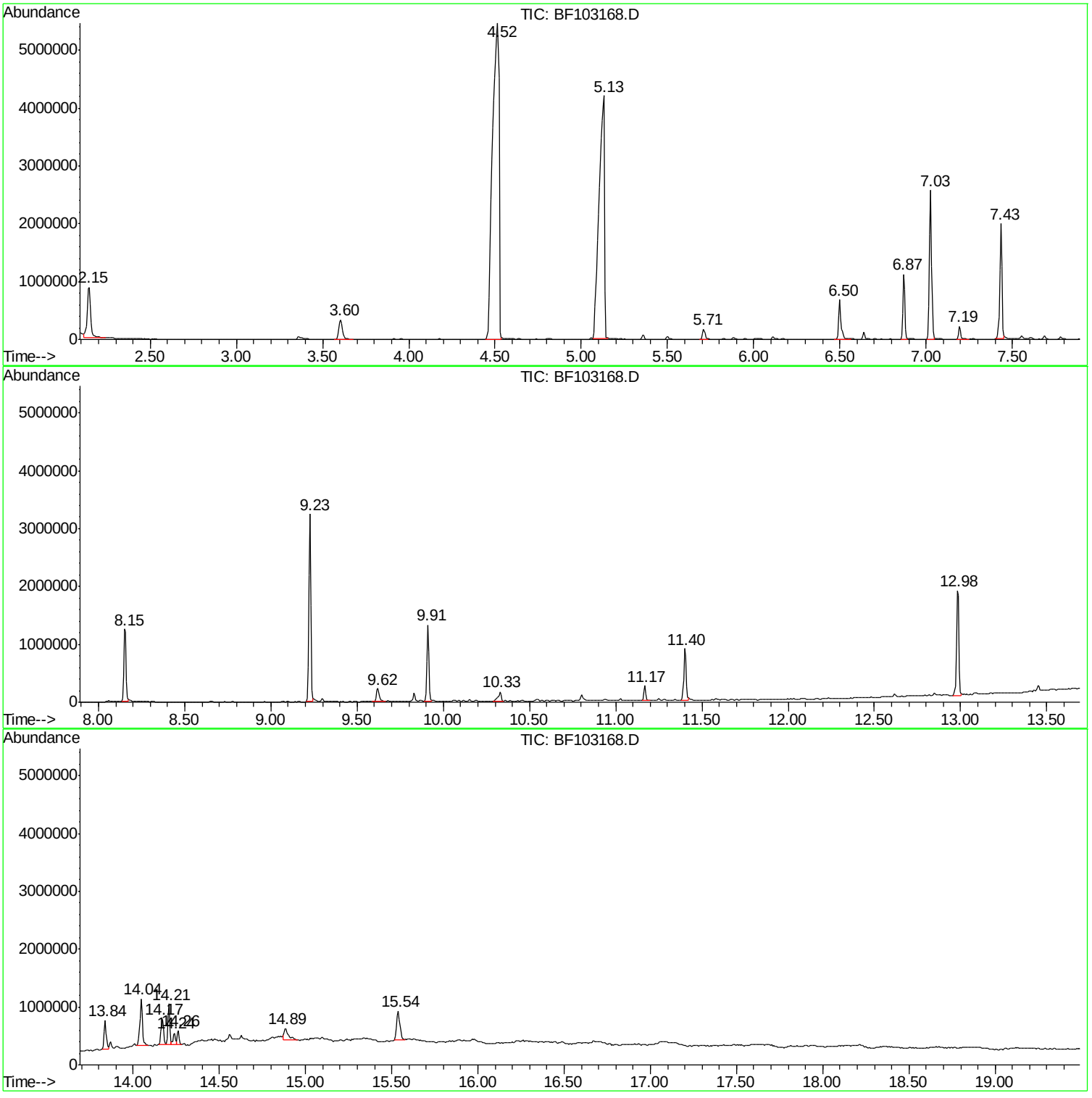
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF022218\
Data File : BF103168.D
Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF103168.D
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Operator : SJ/JU
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

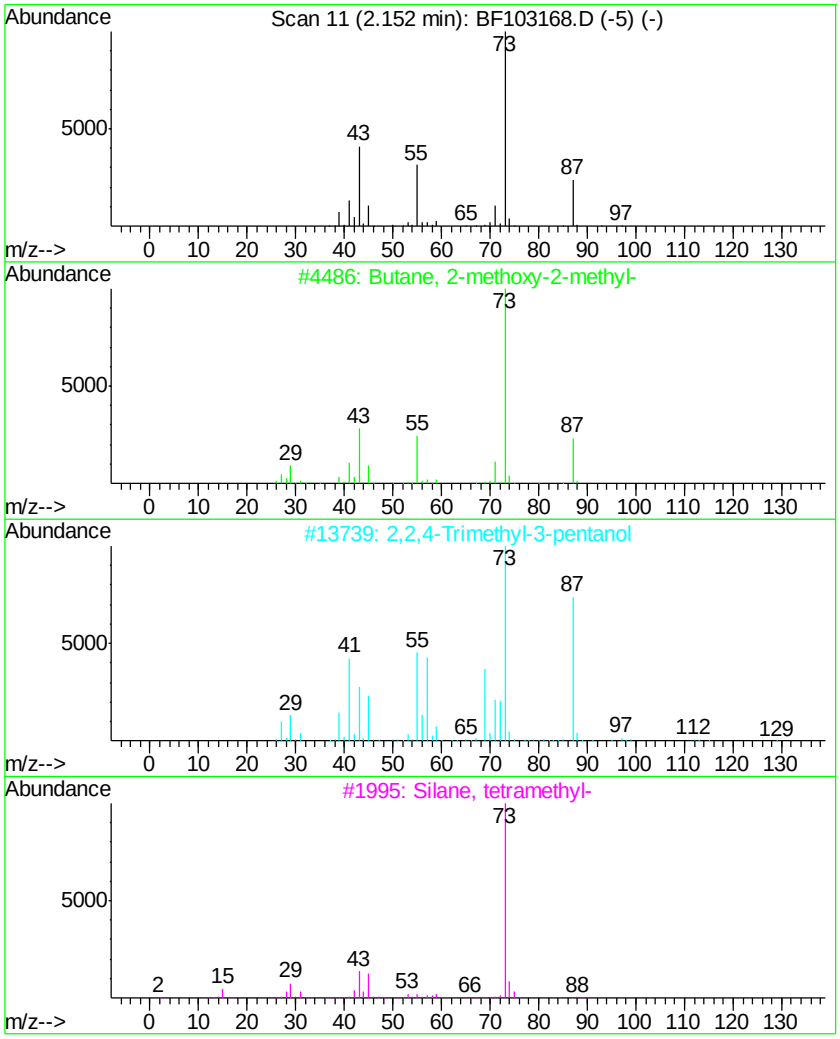
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

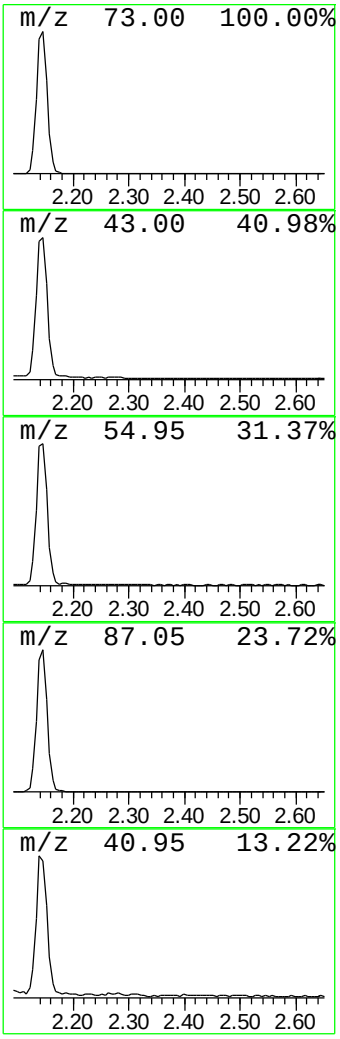
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	26.83 ng	1270160	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

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Data File : BF103168.D
Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

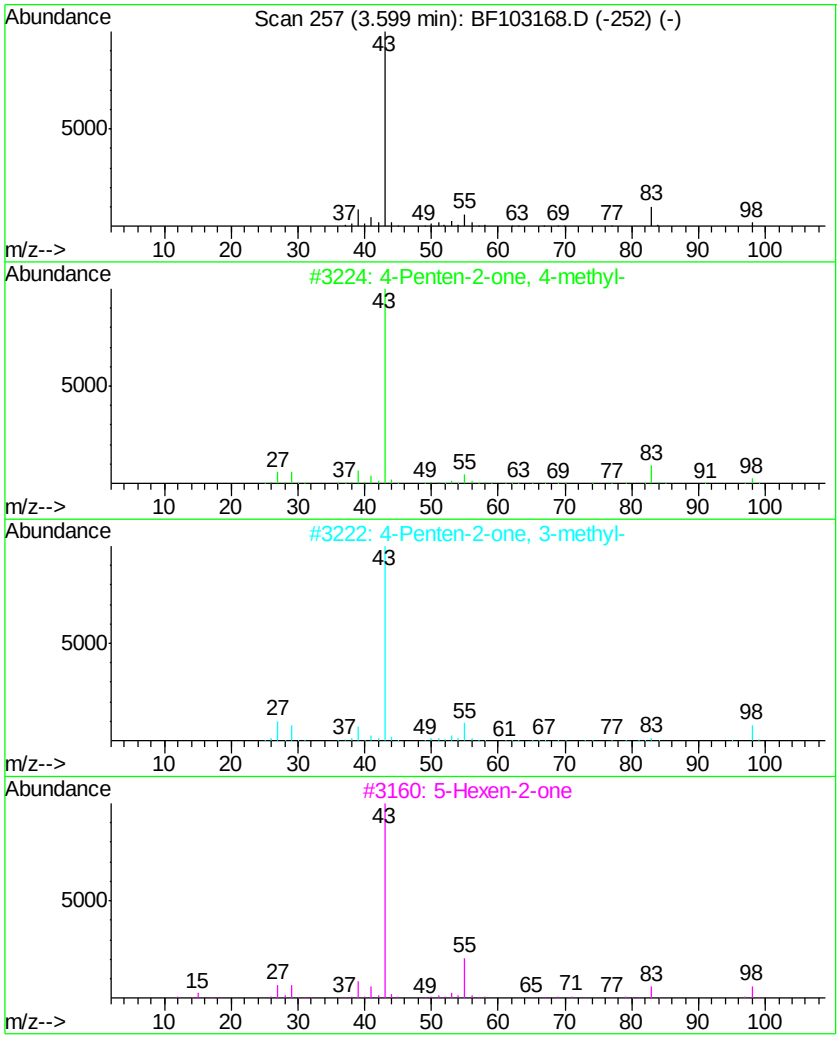
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

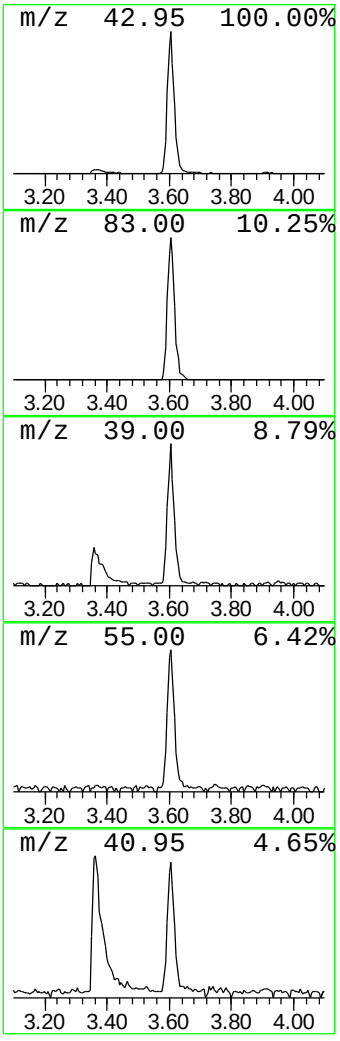
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	11.12 ng	526146	1,4-Dichlorobenzene-d4	6.87

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	40
3	5-Hexen-2-one	98	C6H10O	000109-49-9	38
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	27
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





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Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

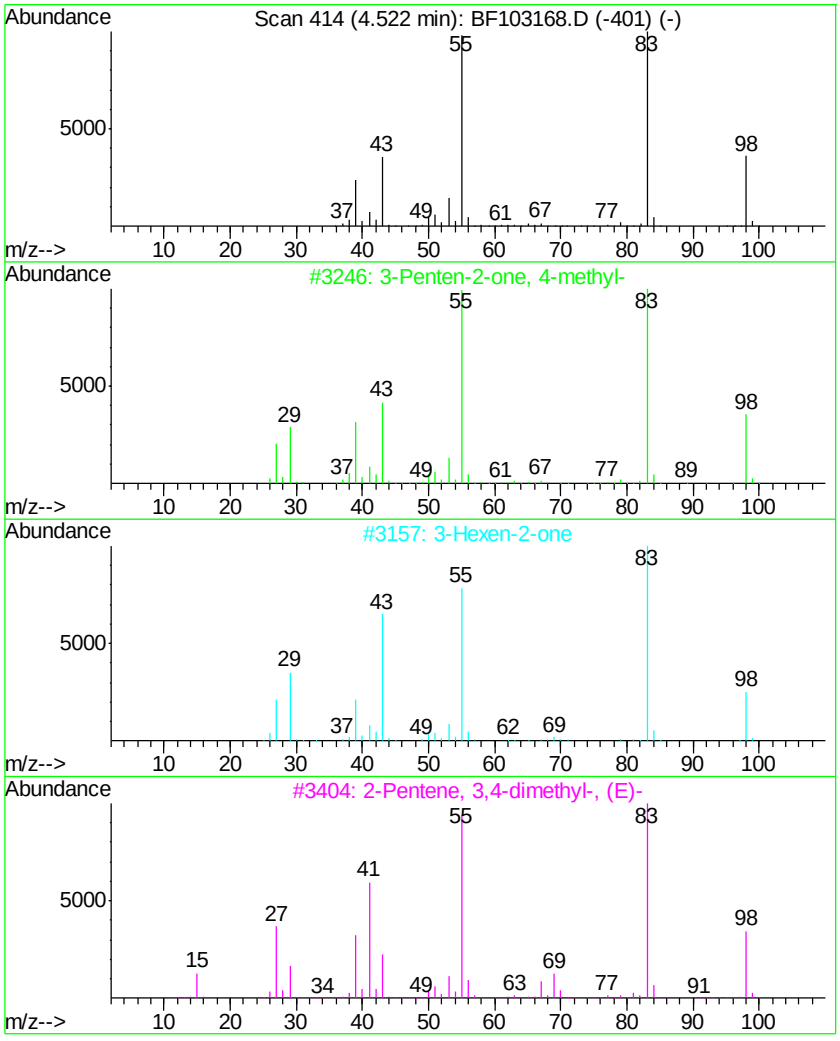
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

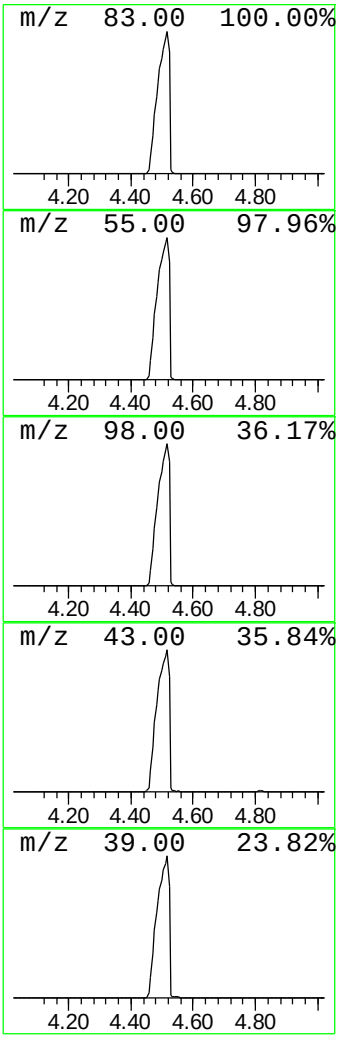
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	301.33 ng	14263600	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Library Search Compound Report

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Data File : BF103168.D
Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

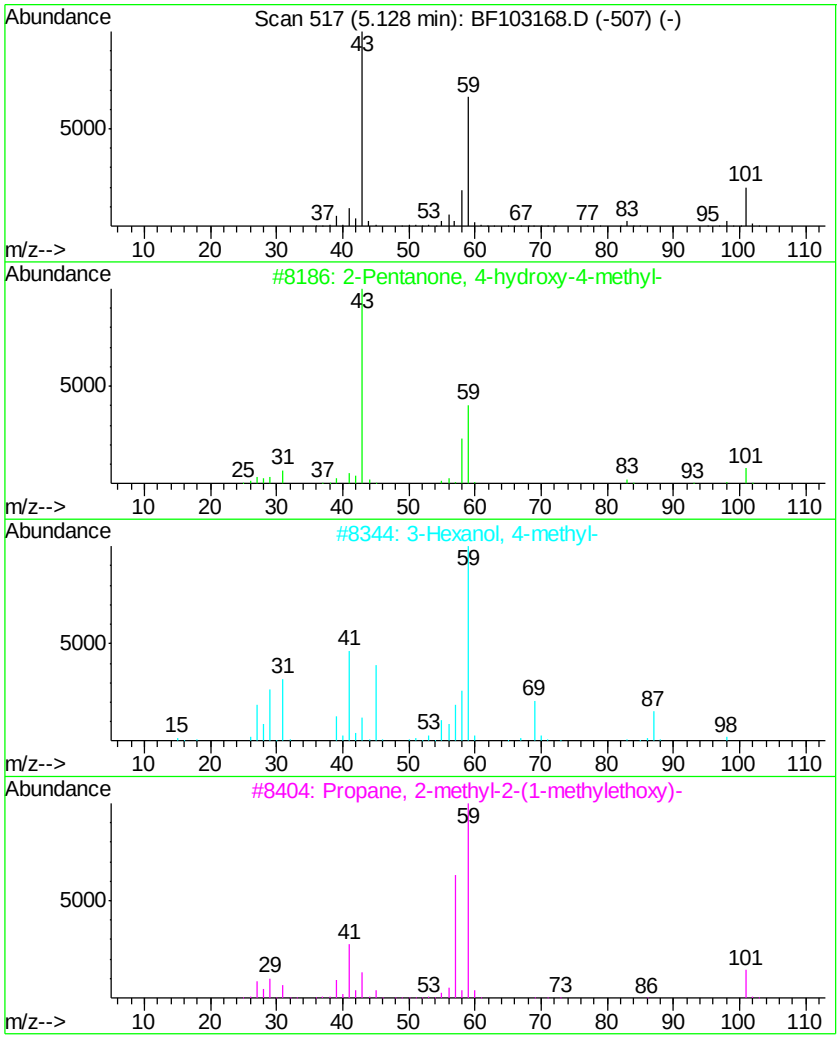
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

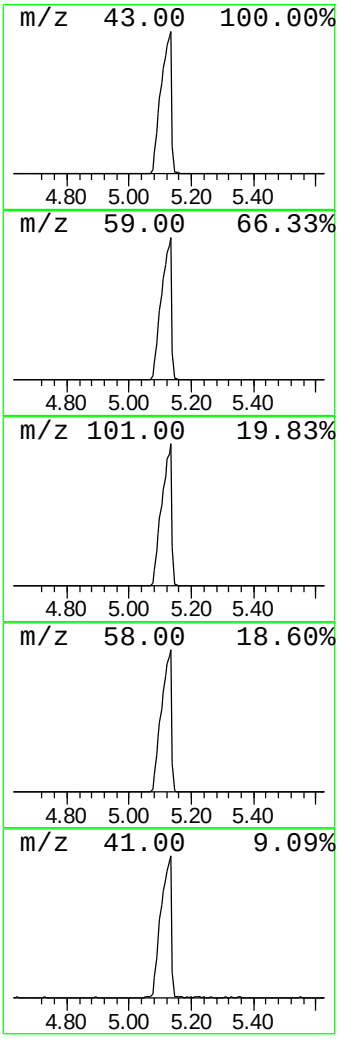
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	205.58 ng	9731100	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	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

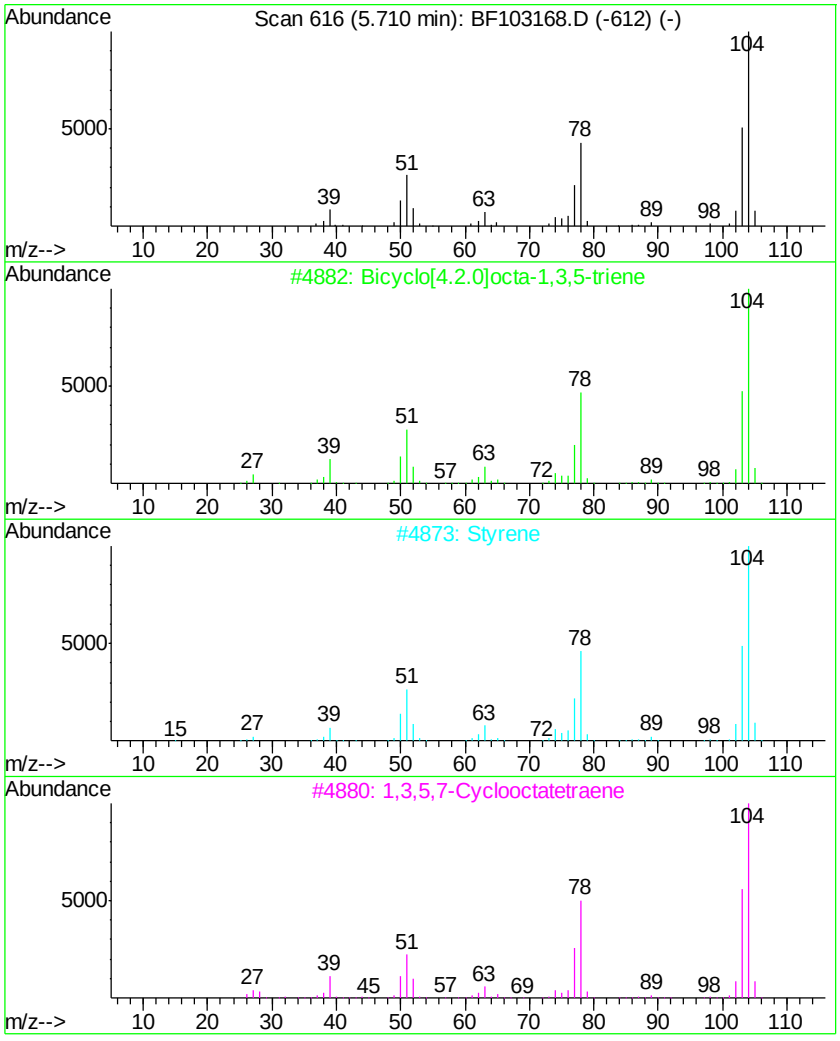
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

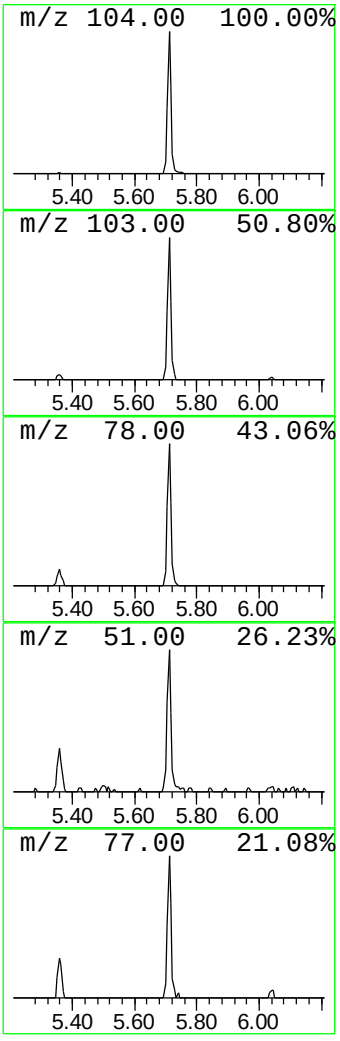
****

Peak Number 5 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	3.11 ng	147394	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
2	Styrene	104	C8H8	000100-42-5	96
3	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	96
4	Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	64
5	1,3,7-Octatrien-5-yne	104	C8H8	016607-77-5	38





Library Search Compound Report

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Data File : BF103168.D
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Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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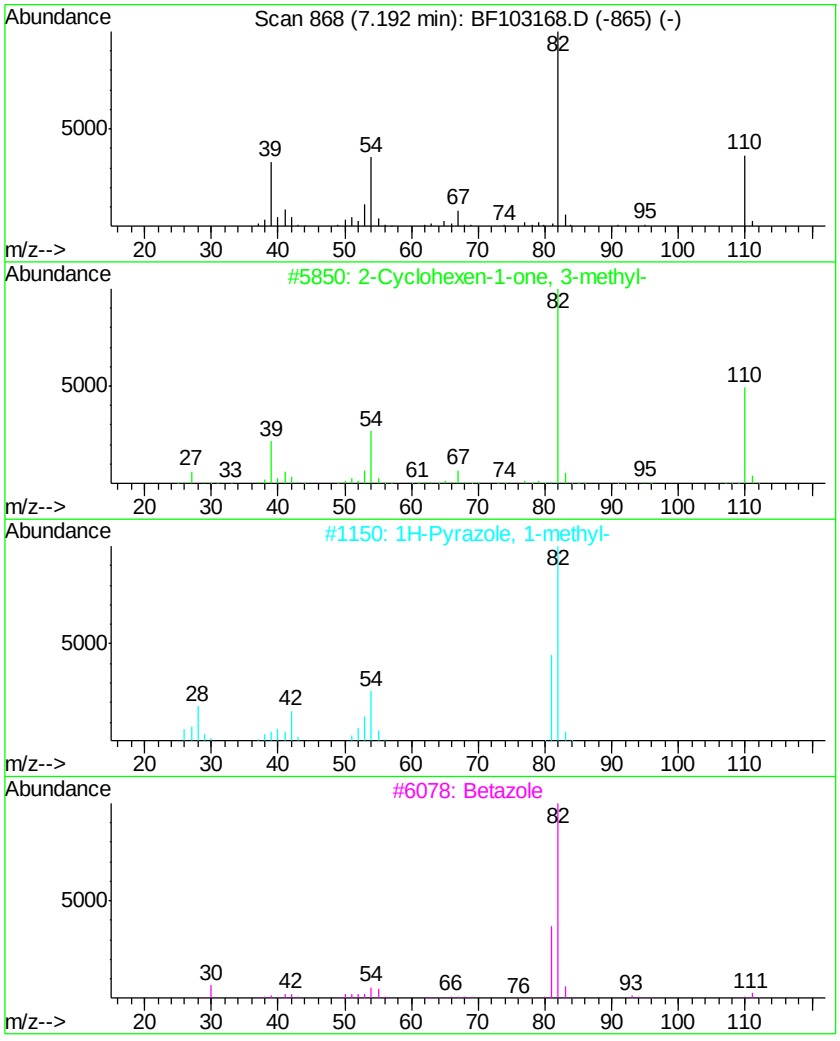
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

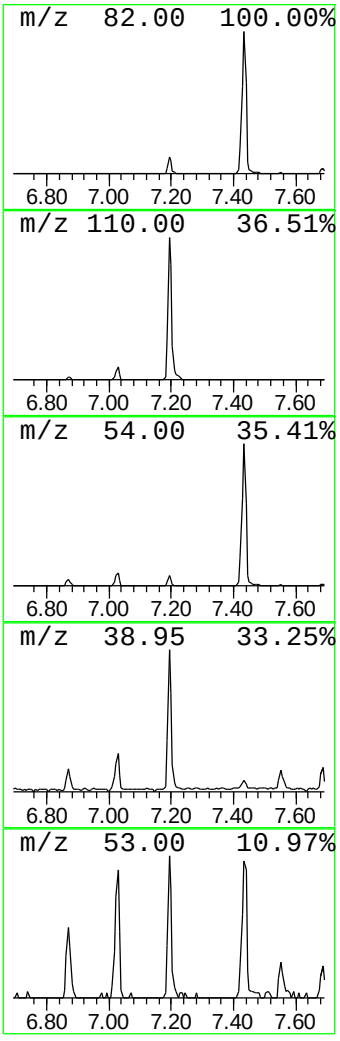
****

Peak Number 7 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	4.07 ng	192518	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	59
3	Betazole	111	C5H9N3	000105-20-4	52
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
5	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	43





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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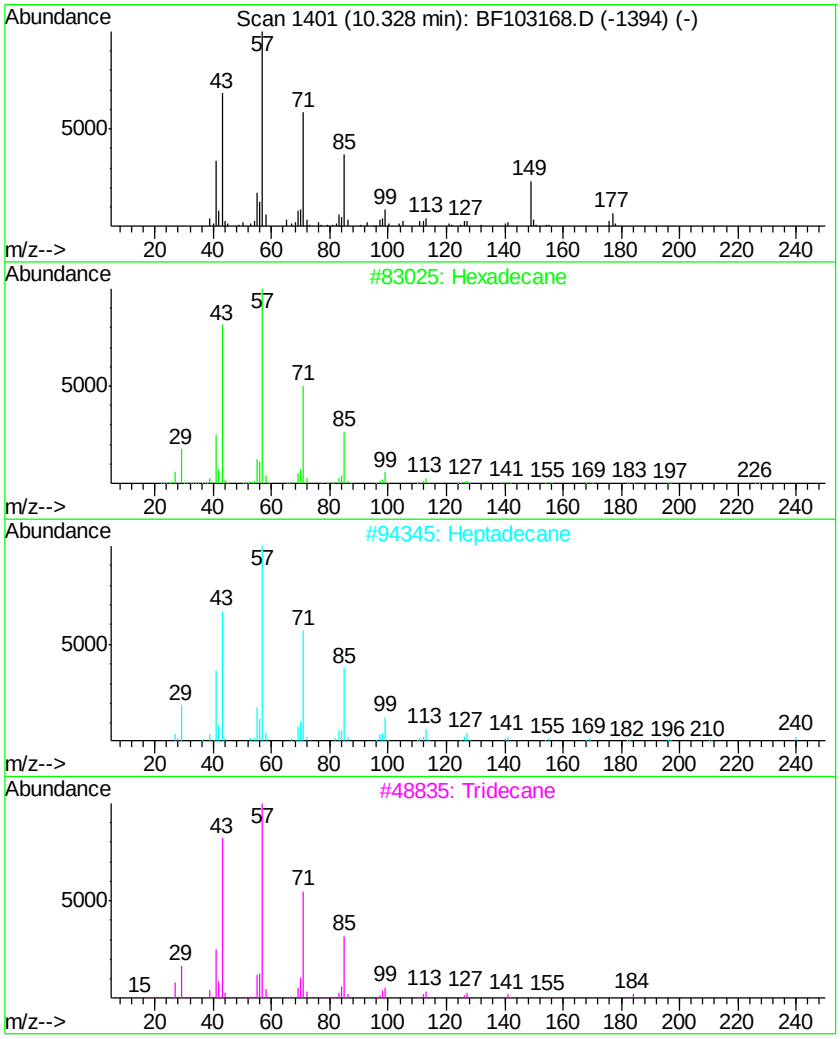
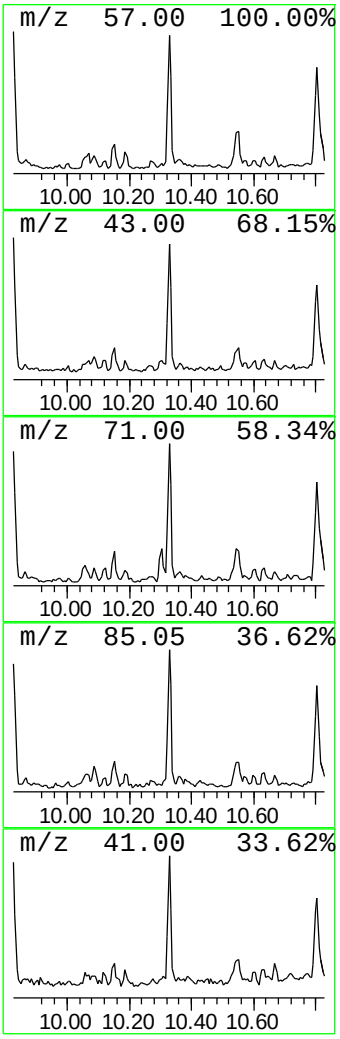
****

Peak Number 8 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	3.34 ng	189327	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	74
2	Heptadecane	240	C17H36	000629-78-7	72
3	Tridecane	184	C13H28	000629-50-5	72
4	Pentadecane	212	C15H32	000629-62-9	72
5	Octadecane	254	C18H38	000593-45-3	64





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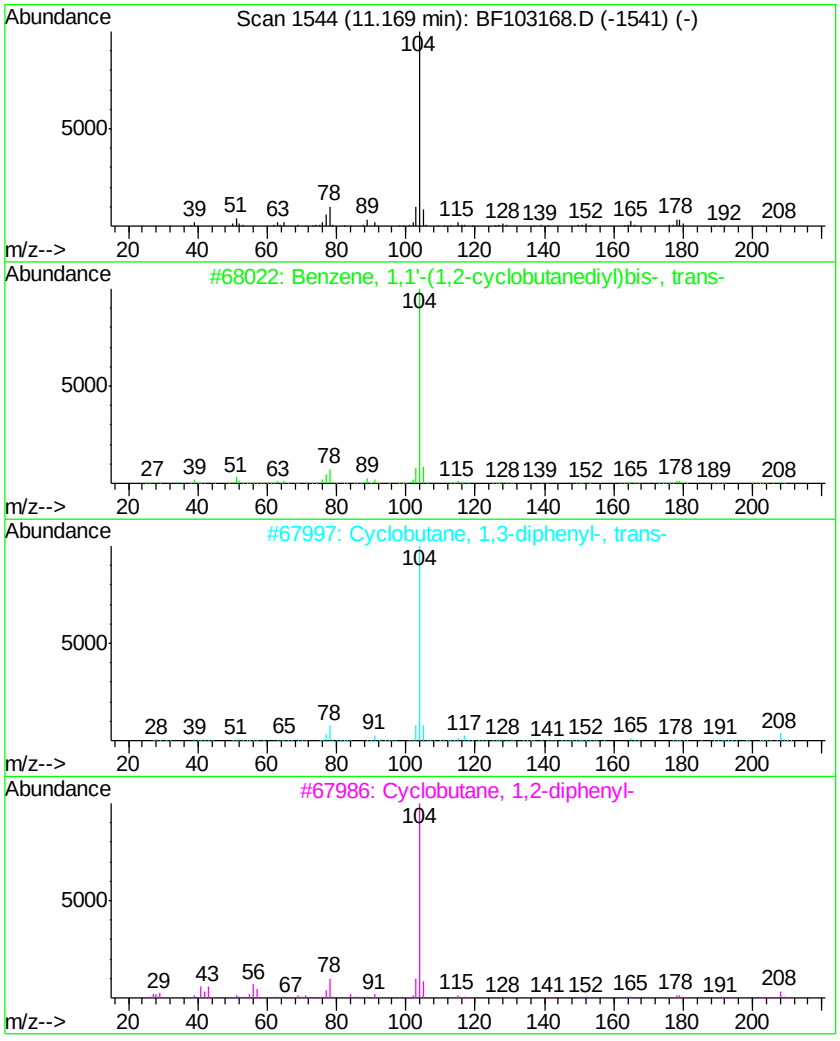
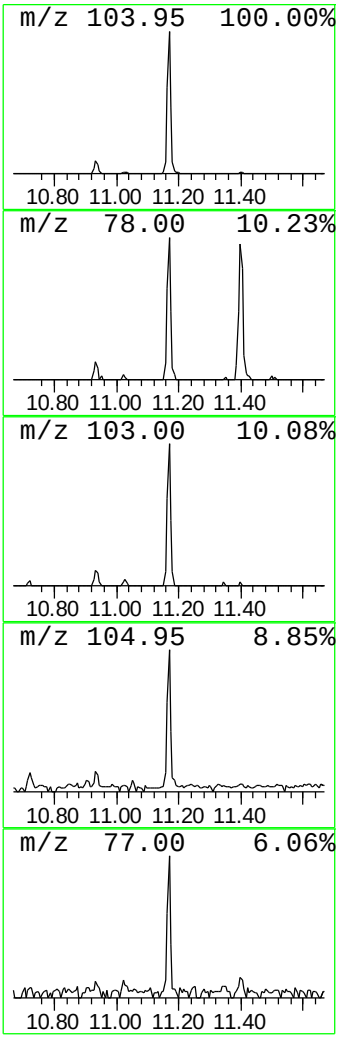
****

Peak Number 9 Benzene, 1,1'-(1,2-cyclobut... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	4.79 ng	203062	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	90
2	Cyclobutane, 1,3-diphenyl-, trans-	208	C16H16	025558-23-0	72
3	Cyclobutane, 1,2-diphenyl-	208	C16H16	003018-21-1	64
4	Styrene	104	C8H8	000100-42-5	64
5	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	64





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

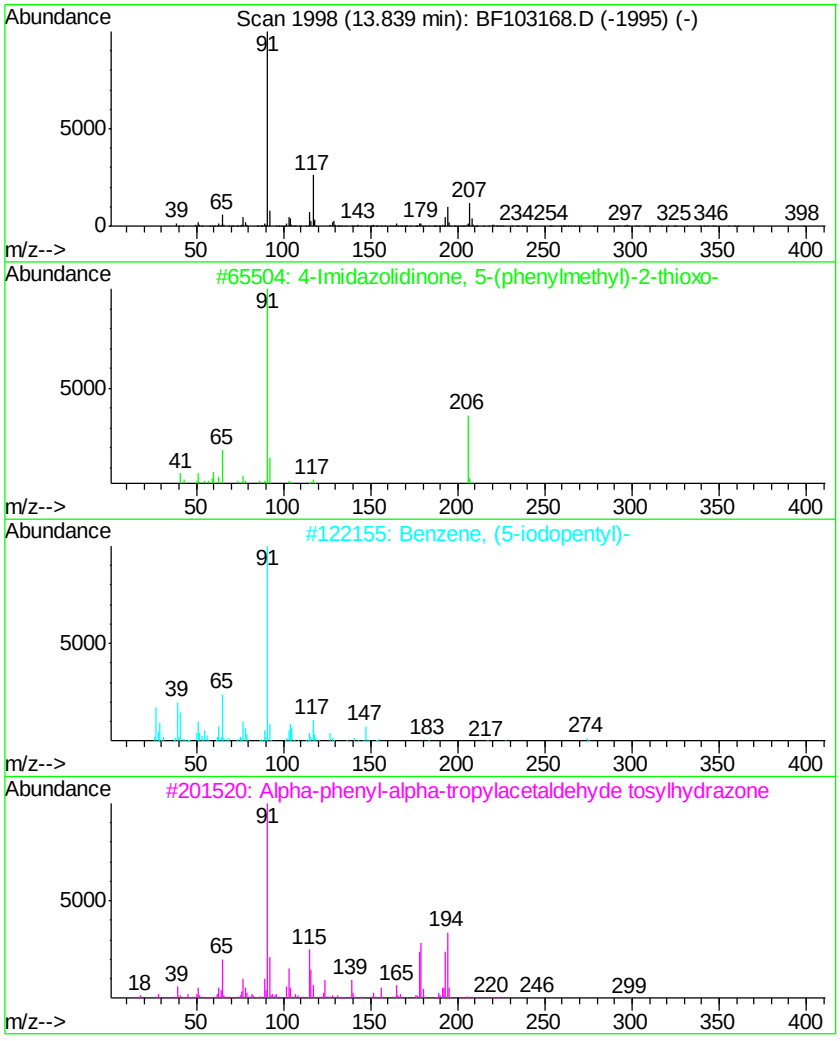
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

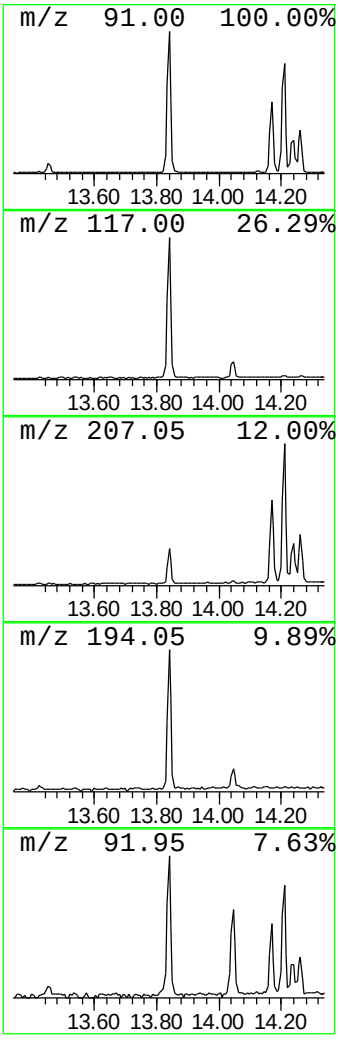
****

Peak Number 10 unknown13.84 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	10.14 ng	413759	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Imidazolidinone, 5-(phenylmeth...	206	C10H10N2OS	006330-09-2	17
2	Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
3	Alpha-phenyl-alpha-tropylacetald...	378	C22H22N2O2S	022532-16-7	16
4	4-Benzyloxy-3-methoxy-2-nitroben...	303	C15H13NO6	003584-32-5	10
5	Benzene, 1-methyl-4-[(phenylmeth...	246	C14H14O2S	005395-20-0	10





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Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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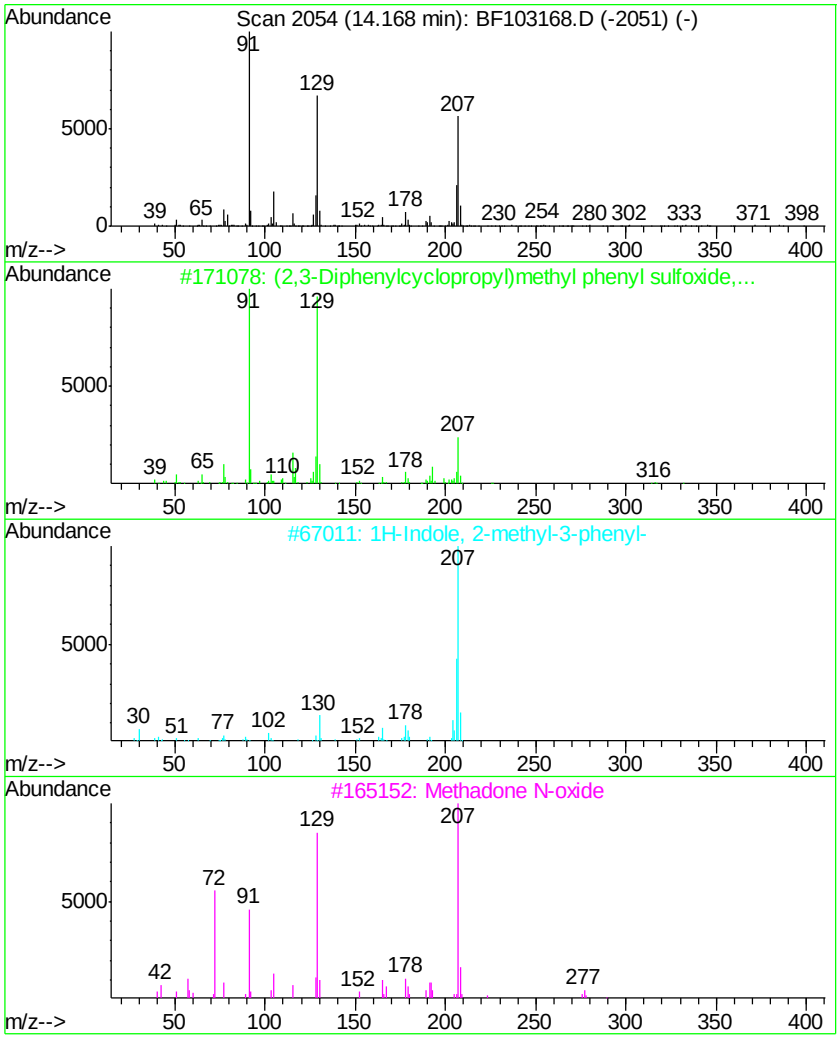
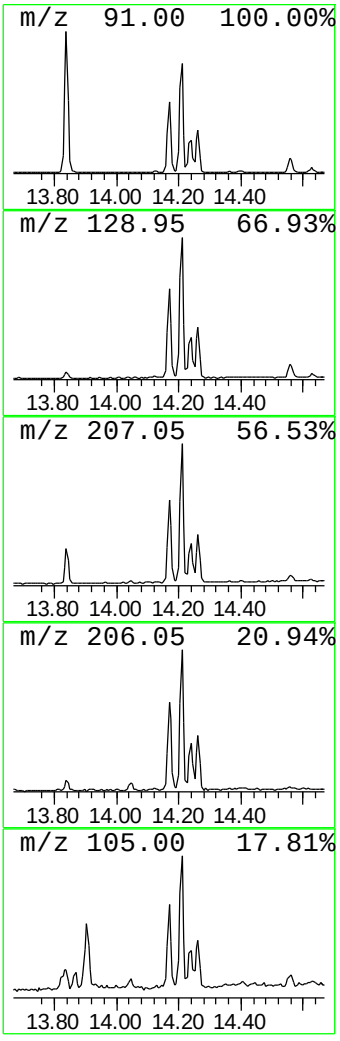
Peak Number 11 (2,3-Diphenylcyclopropyl)me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	9.38 ng	382856	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	50
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	43
3	Methadone N-oxide	325	C21H27NO2	1000120-80-7	42
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38
5	1-benzylindole	207	C15H13N	1000334-31-3	35





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Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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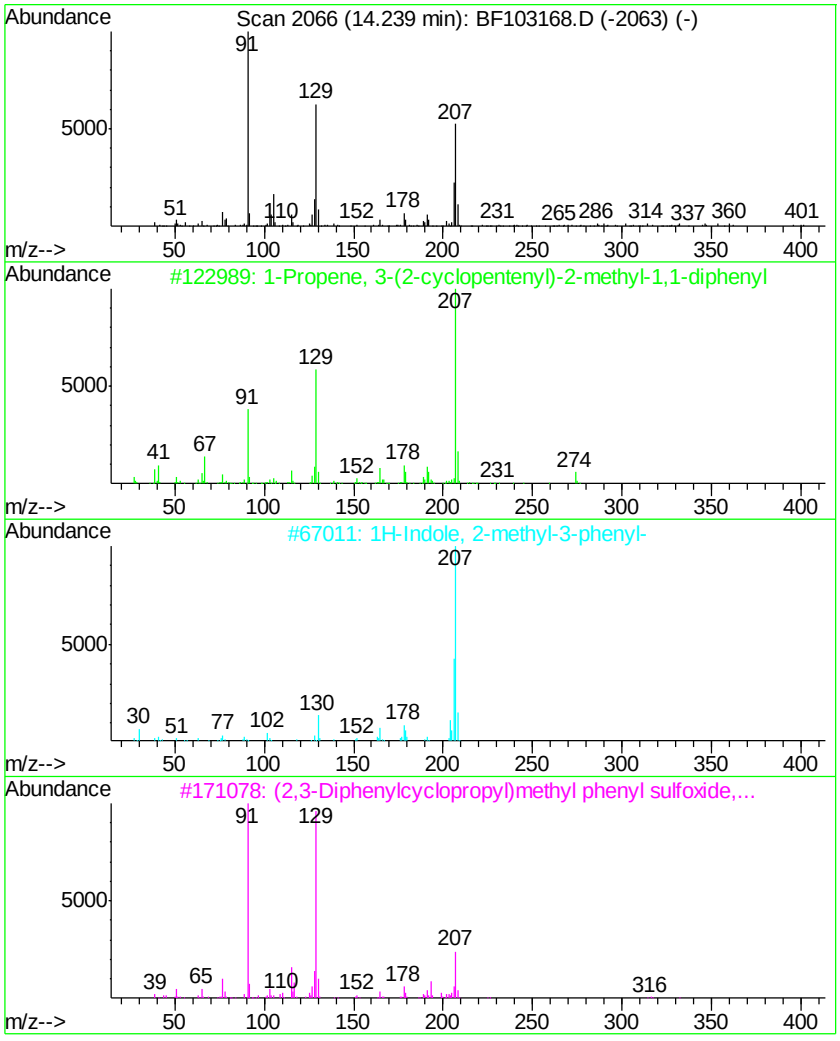
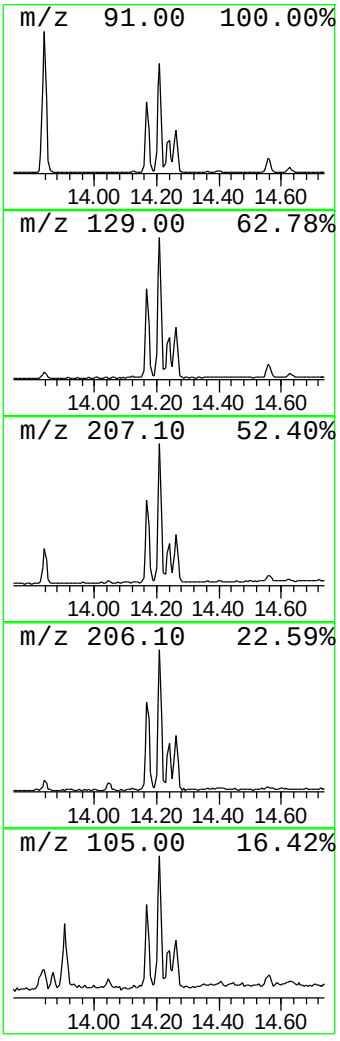
Peak Number 13 1-Propene, 3-(2-cyclopenten... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	4.74 ng	193286	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	59
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38
3	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	38
4	1-benzylindole	207	C15H13N	1000334-31-3	35
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	35





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Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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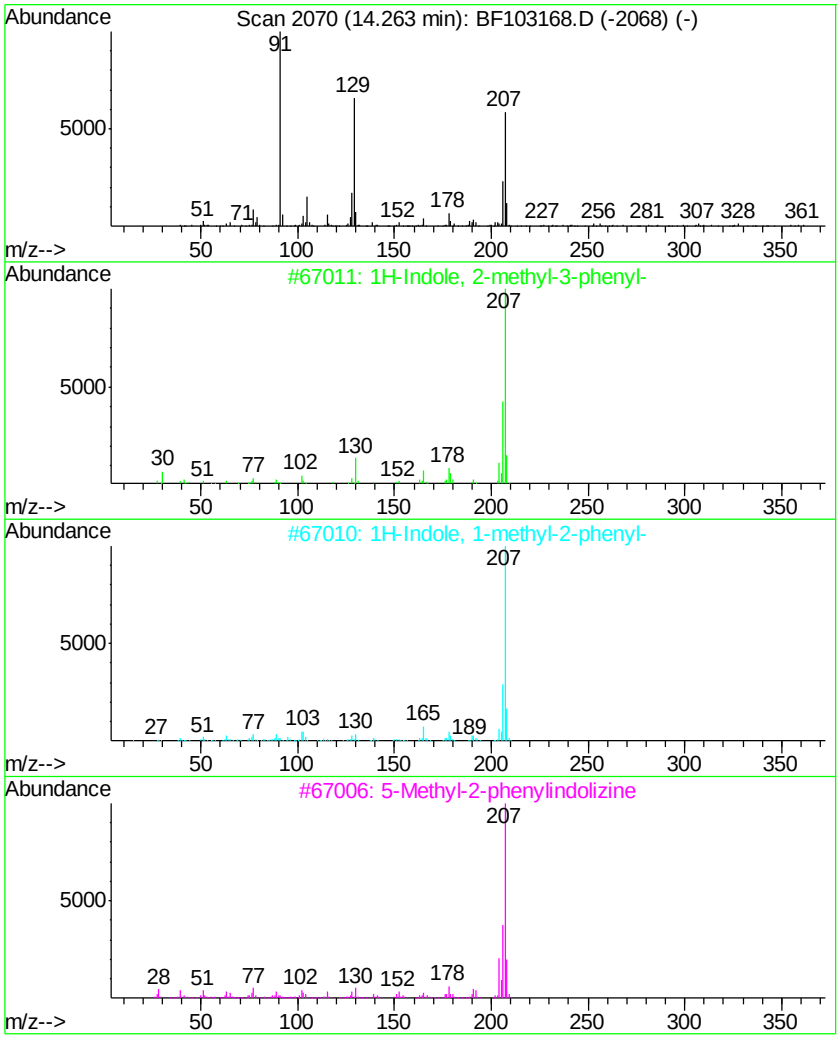
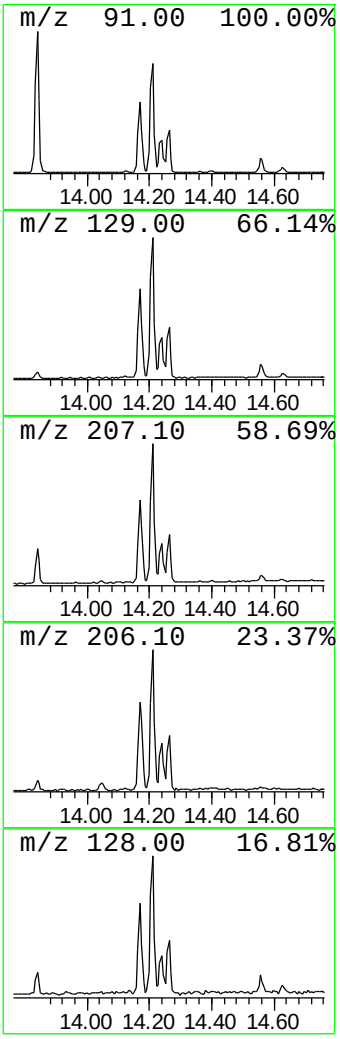
Peak Number 14 unknown14.26 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	4.44 ng	180983	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	43
2	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	41
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38
4	1-benzylindole	207	C15H13N	1000334-31-3	35
5	2-[2-[2-(4-Chloro-phenoxy)-ethyl...	361	C17H16ClN3O2S	1000296-99-3	35





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Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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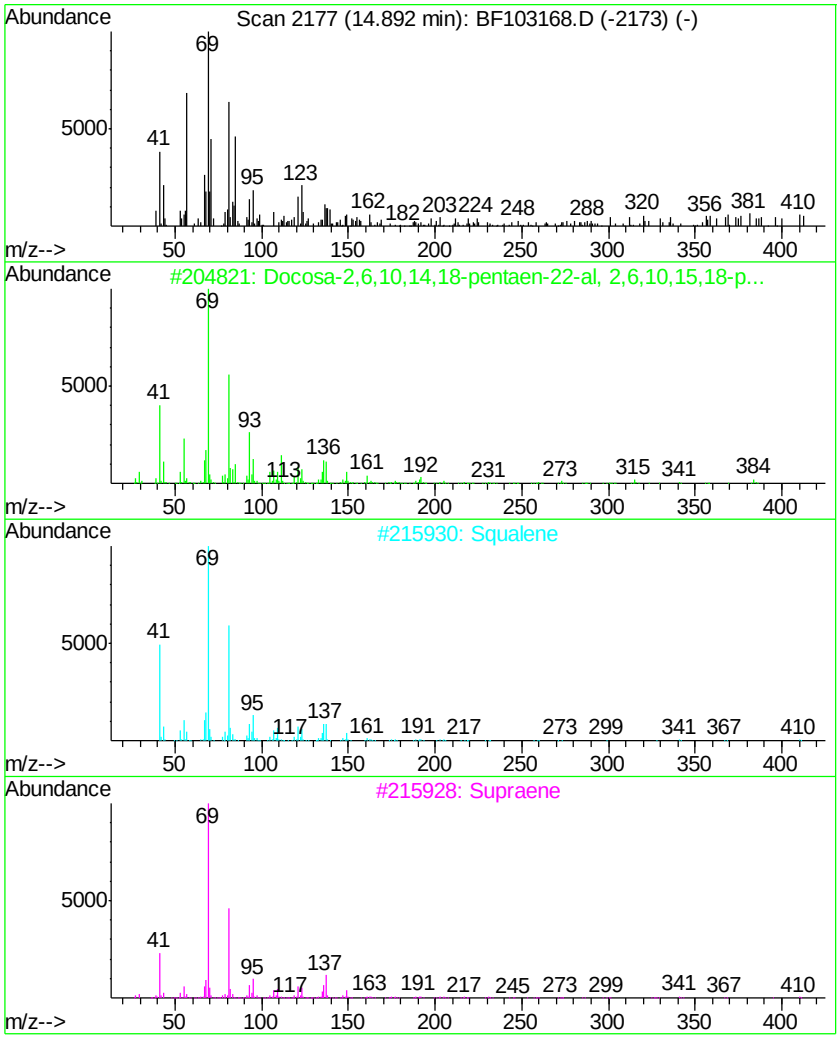
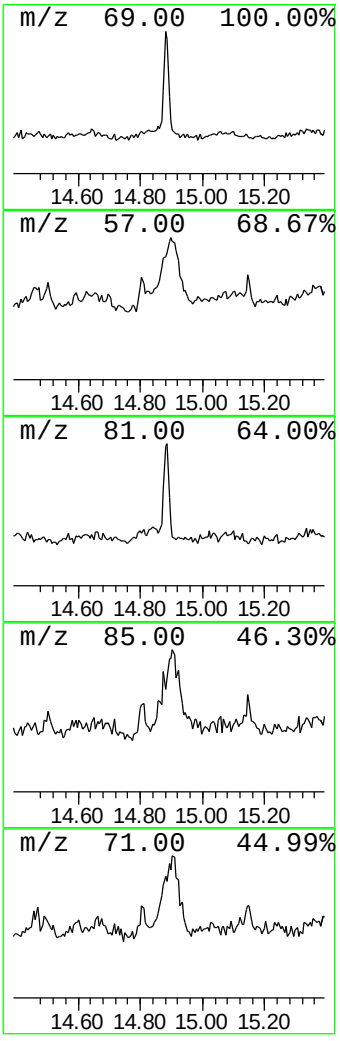
Peak Number 15 Docosa-2,6,10,14,18-pentaen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	12.14 ng	385047	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
2	Squalene	410	C30H50	000111-02-4	83
3	Supraene	410	C30H50	007683-64-9	80
4	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
5	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	64





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF022218\
Data File : BF103168.D
Acq On : 22 Feb 2018 17:56
Operator : SJ/JU
Sample : J1639-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSE-GRADE-AGG-RCA

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	26.8	ng	1270160	1	6.87	946714	20.0
4-Penten-2-one, 4...	3.60	11.1	ng	526146	1	6.87	946714	20.0
3-Penten-2-one, 4...	4.52	301.3	ng	14263600	1	6.87	946714	20.0
2-Pentanone, 4-hy...	5.13	205.6	ng	9731100	1	6.87	946714	20.0
Bicyclo[4.2.0]oct...	5.71	3.1	ng	147394	1	6.87	946714	20.0
2-Cyclohexen-1-on...	7.19	4.1	ng	192518	1	6.87	946714	20.0
Hexadecane	10.33	3.3	ng	189327	3	9.91	1133160	20.0
Benzene, 1,1'-(1,...	11.17	4.8	ng	203062	4	11.40	848208	20.0
unknown13.84	13.84	10.1	ng	413759	5	14.04	815908	20.0
(2,3-Diphenylcycl...	14.17	9.4	ng	382856	5	14.04	815908	20.0
1-Propene, 3-(2-c...	14.24	4.7	ng	193286	5	14.04	815908	20.0
unknown14.26	14.26	4.4	ng	180983	5	14.04	815908	20.0
Docosa-2,6,10,14,...	14.89	12.1	ng	385047	6	15.54	634323	20.0