LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

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-BF102616.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	2.144	3	5	14	rVB3	60008	189352	3.23%	0.305%
2	3.550	123	128	130	rBV	29118	74442	1.27%	0.120%
3	3.721	139	143	149	rVB	59030	143500	2.45%	0.231%
4	4.007	163	168	170	rBV	31233	59561	1.02%	0.096%
5	4.258	183	190	198	rBV2	117370	267738	4.56%	0.431%
6	4.899	244	246	253	rBV	762646	1344956	22.93%	2.166%
7	5.299	277	281	282	rBV	68348	87370	1.49%	0.141%
8	5.333	282	284	287	rBV	4114386	5243809	89.39%	8.445%
9	5.470	293	296	303	rVB2	53763	112569	1.92%	0.181%
10	5.630	303	310	313	rVB3	88563	149222	2.54%	0.240%
11	6.384	373	376	379	rBV	4058704	5091712	86.80%	8.200%
12	6.510	384	387	389	rBV	4931533	5866099	100.00%	9.447%
13	6.739	405	407	409	rBV	982472	1065345	18.16%	1.716%
14	6.887	418	420	423	rBV	3043345	4238163	72.25%	6.825%
15	7.310	454	457	459	rBV	2723778	3702822	63.12%	5.963%
16	7.413	463	466	468	rVV	132462	138893	2.37%	0.224%
17	8.019	517	519	522	rBV	1391806	1465109	24.98%	2.359%
18	8.316	541	545	546	rBV3	38079	66639	1.14%	0.107%
19	8.373	549	550	552	rBV	42535	67351	1.15%	0.108%
20	8.453	555	557	562	rBV3	81695	177040	3.02%	0.285%
21	8.567	565	567	571	rBV	111913	147109	2.51%	0.237%
22	8.682	573	577	579	rVV5	29876	80937	1.38%	0.130%
23	8.762	583	584	586	rBV	49865	63213	1.08%	0.102%
24	8.910	595	597	598	rBV	63714	67281	1.15%	0.108%
25	9.013	604	606	607	rBV	91246	71159	1.21%	0.115%
26	9.059	607	610	611	rVB	120421	148527	2.53%	0.239%
27	9.105	611	614	616	rBV	5816437	5590975	95.31%	9.004%
28	9.185	618	621	624	rBV	170386	249886	4.26%	0.402%
29	9.505	645	649	651	rBV	970931	1490478	25.41%	2.400%
30	9.653	660	662	664	rBV2	107043	186770	3.18%	0.301%
31	9.688	664	665	666	rVV	211910	159310	2.72%	0.257%
32	9.722	666	668	669	rVV	162213	167375	2.85%	0.270%
33	9.779	669	673	674	rVV	1490636	1837177	31.32%	2.959%
34	9.802	674	675	679	rVB3	78054	186172	3.17%	0.300%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

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-BF102616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.939	685	687	689	rBV2	84768	141697	2.42%	0.228%
36	10.042	694	696	697	rBV	222727	222418	3.79%	0.358%
37	10.110	700	702	703	rBV2	104636	141142	2.41%	0.227%
38	10.179	706	708	710	rBV2	141235	162914	2.78%	0.262%
39	10.213	710	711	715	rBV	171531	337424	5.75%	0.543%
40	10.442	728	731	733	rBV	361564	389436	6.64%	0.627%
41	10.568	739	742	744	rBV	3132357	3334235	56.84%	5.370%
42	10.625	744	747	748	rVB2	138021	194657	3.32%	0.313%
43	10.705	751	754	757	rVV	565526	1013983	17.29%	1.633%
44	11.139	791	792	793	rBV	307388	281111	4.79%	0.453%
45	11.173	793	795	797	rVB	397145	460902	7.86%	0.742%
46	11.253	800	802	805	rBV	948121	1377359	23.48%	2.218%
47	12.854	940	942	945	rBV	2940981	3096048	52.78%	4.986%
48	15.974	1212	1215	1223	rVB	1556958	4332987	73.86%	6.978%
49	16.363	1246	1249	1256	rVB	2001899	4075329	69.47%	6.563%
50	16.877	1292	1294	1297	rVV	653536	1099344	18.74%	1.770%
51	16.945	1298	1300	1308	rVB2	668330	1435958	24.48%	2.313%

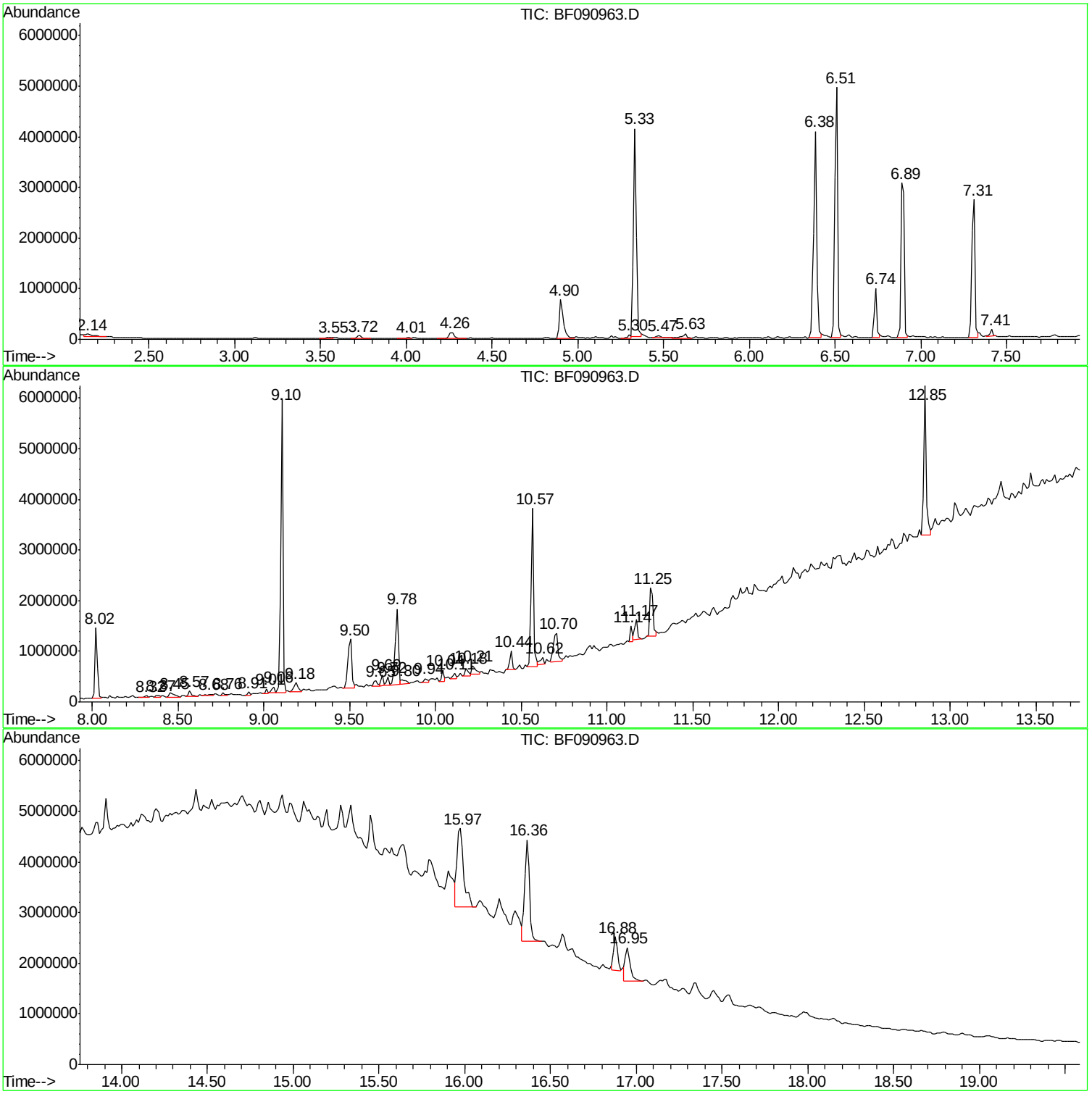
Sum of corrected areas: 62095005

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

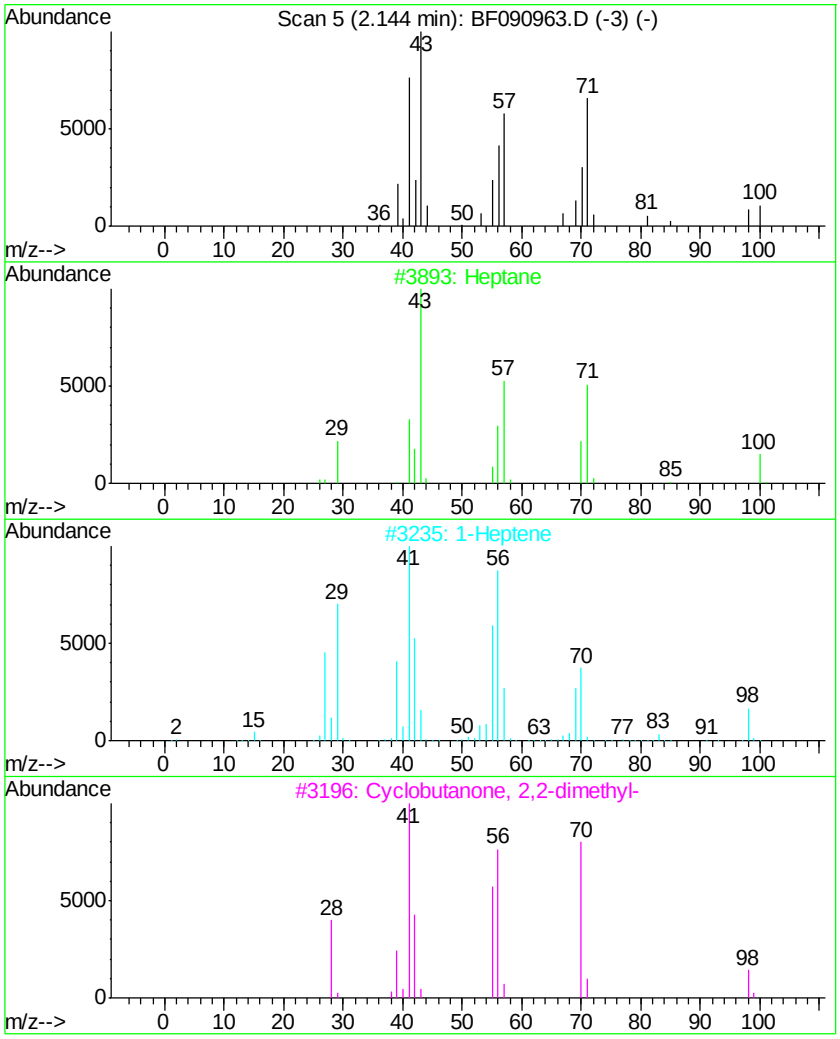
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

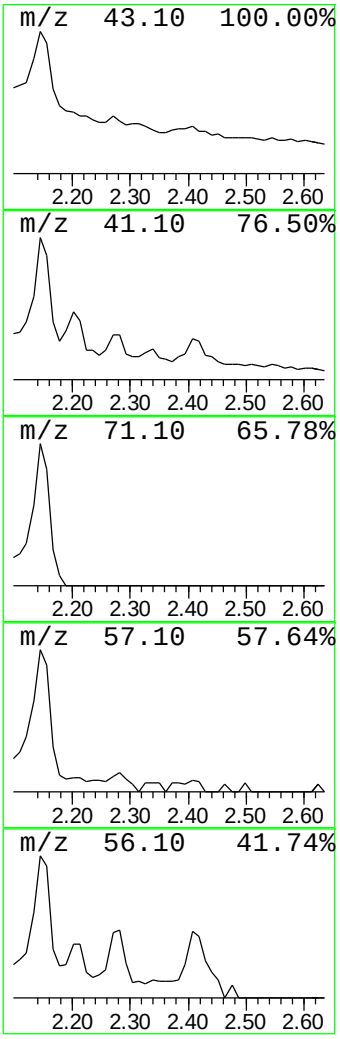
****

Peak Number 1 Heptane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	3.55 ng	189352	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	72
2	1-Heptene	98	C7H14	000592-76-7	43
3	Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	43
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

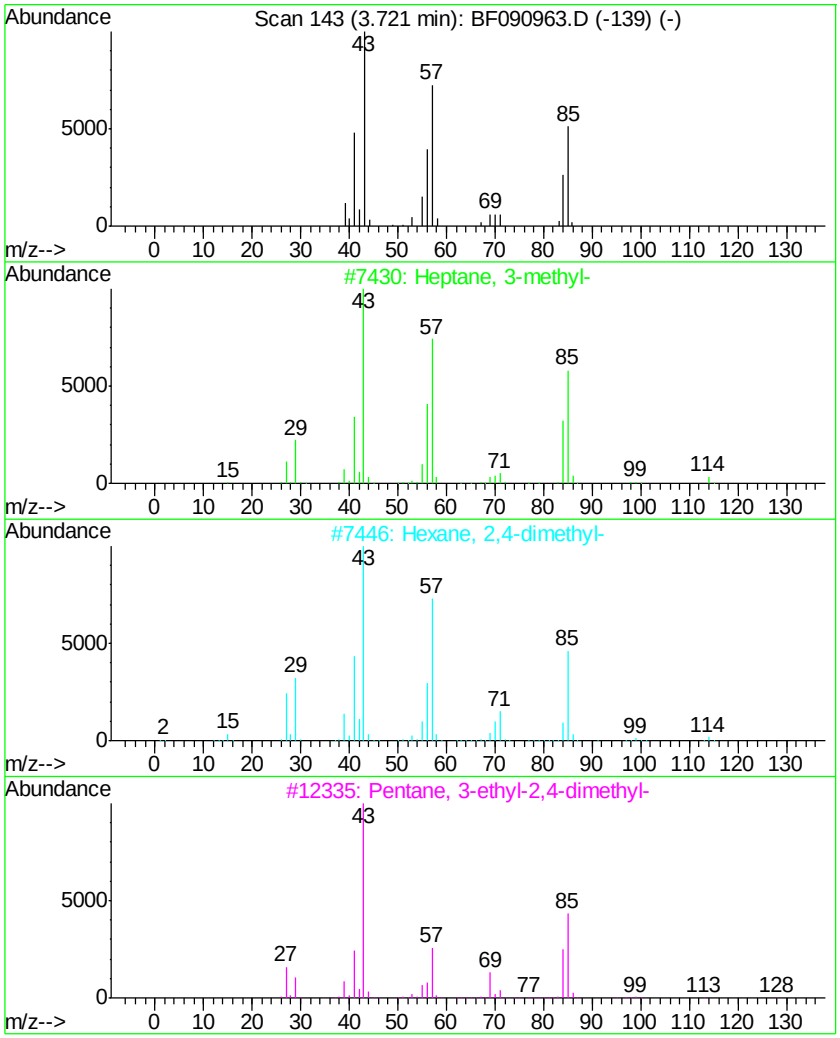
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

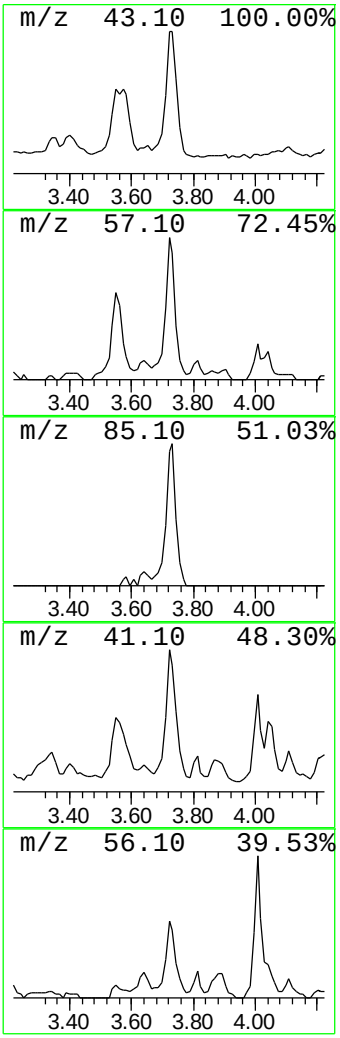
****

Peak Number 2 Heptane, 3-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	2.69 ng	143500	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	83
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59
3	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53
5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

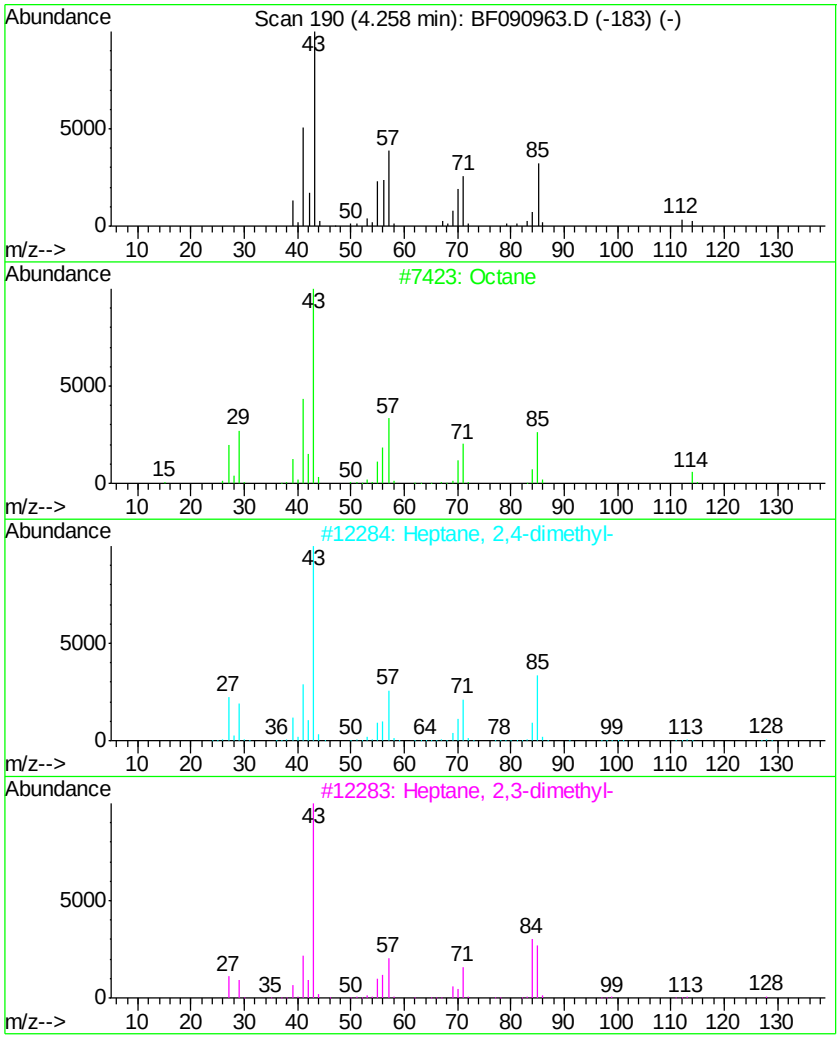
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

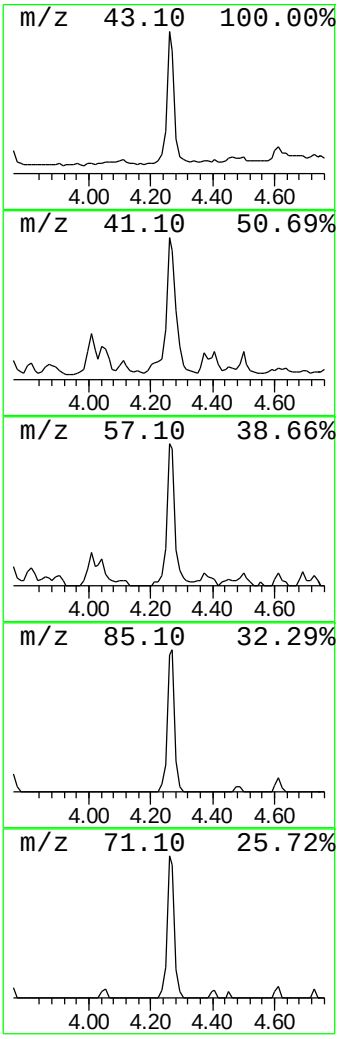
****

Peak Number 3 Octane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	5.03 ng	267738	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	78
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	59
4	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	53
5	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

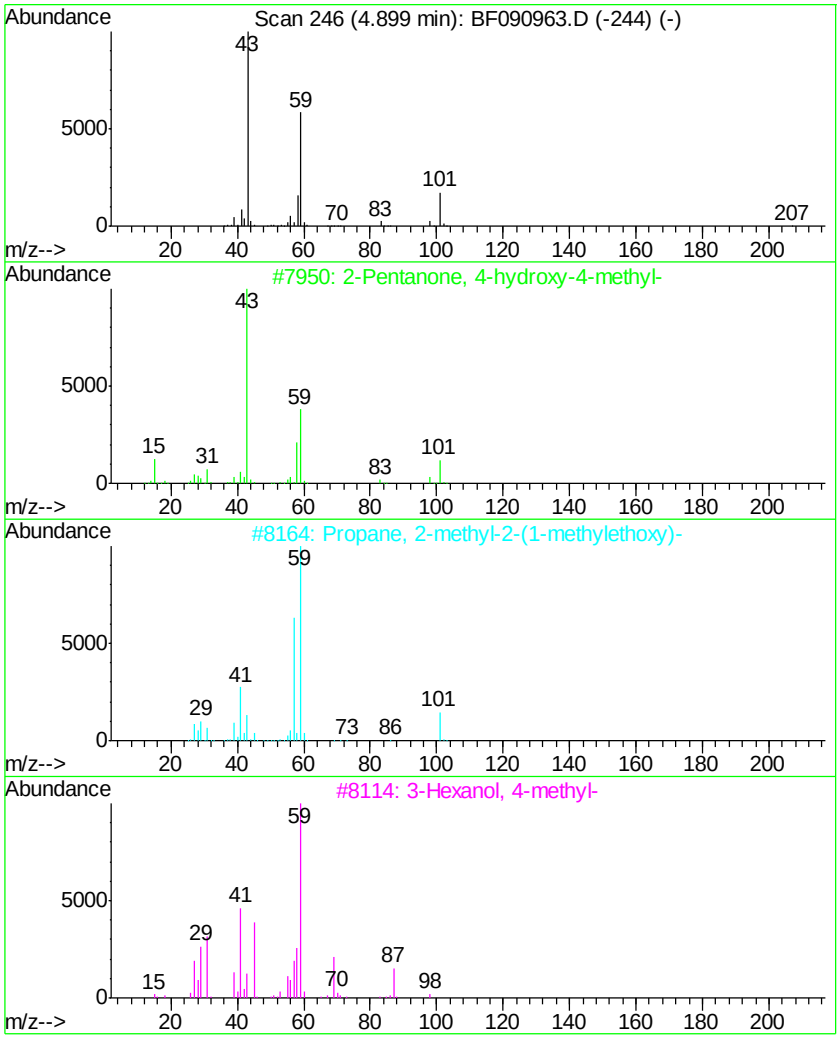
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

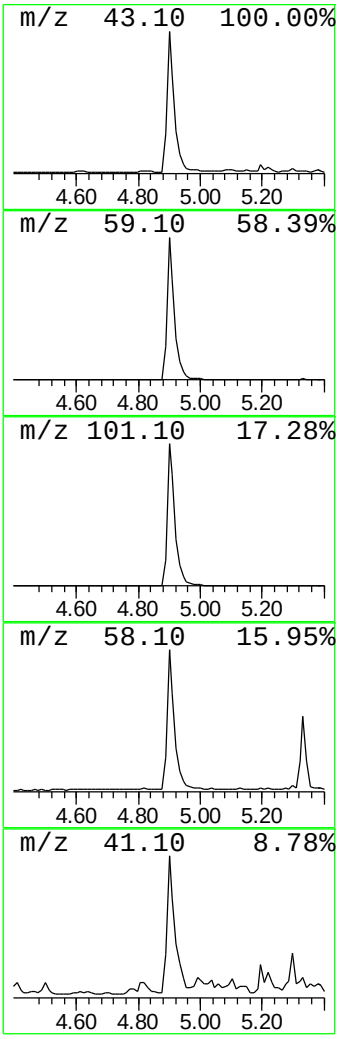
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	25.25 ng	1344960	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
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\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

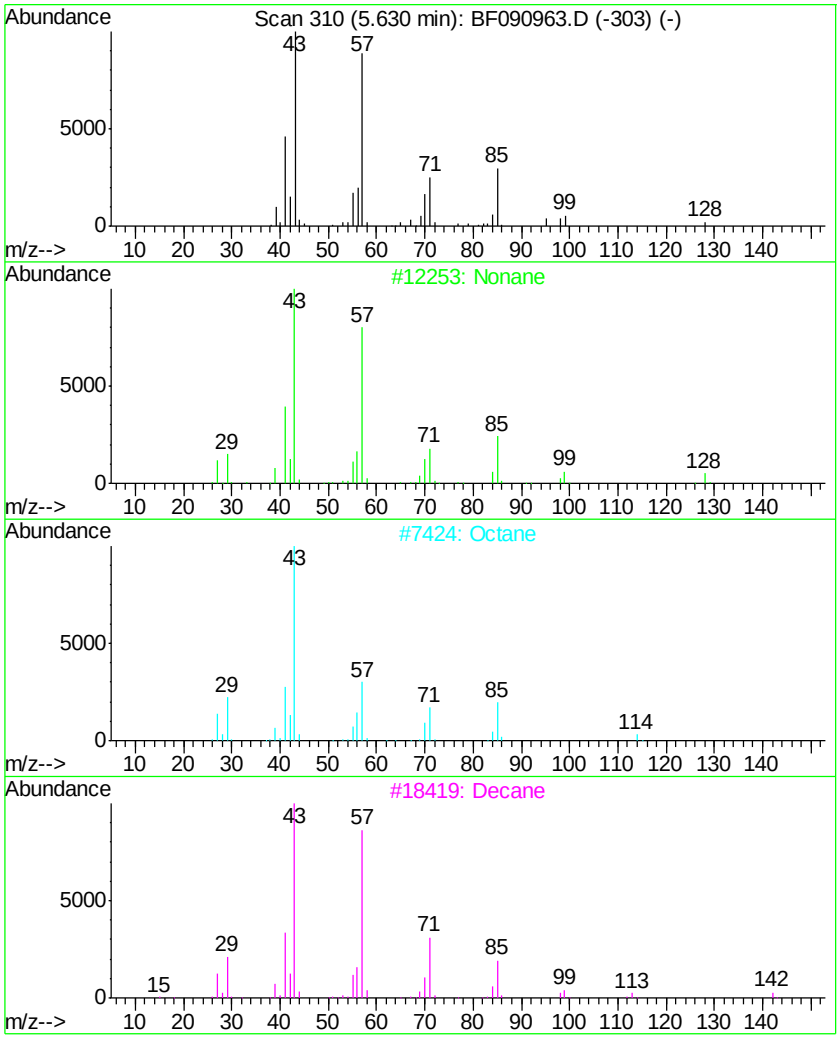
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

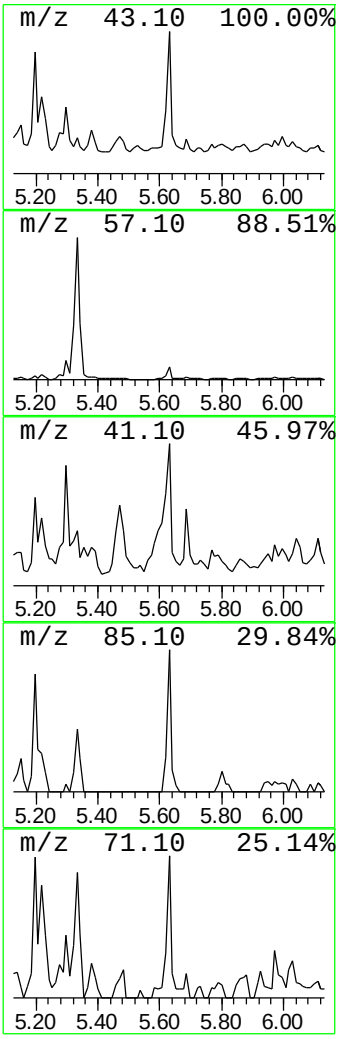
****

Peak Number 5 Nonane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	2.80 ng	149222	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	91
2	Octane	114	C8H18	000111-65-9	64
3	Decane	142	C10H22	000124-18-5	64
4	Octane, 4-methyl-	128	C9H20	002216-34-4	52
5	Dodecane, 5-methyl-	184	C13H28	017453-93-9	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

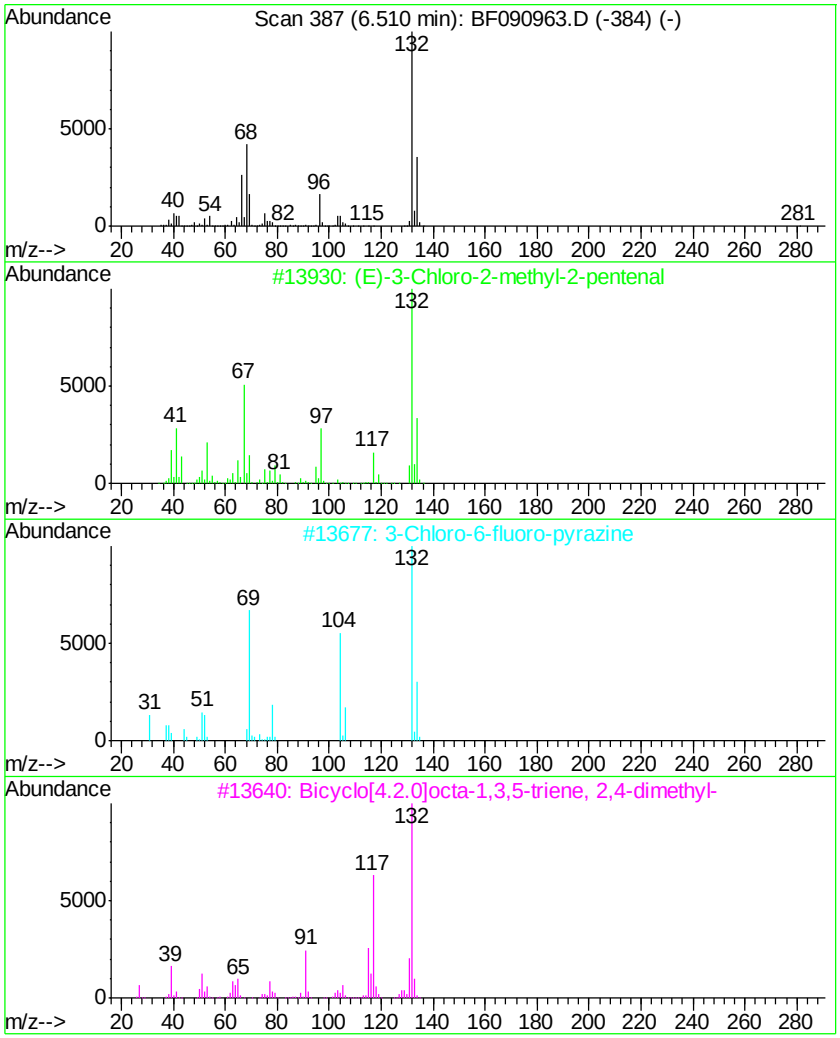
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

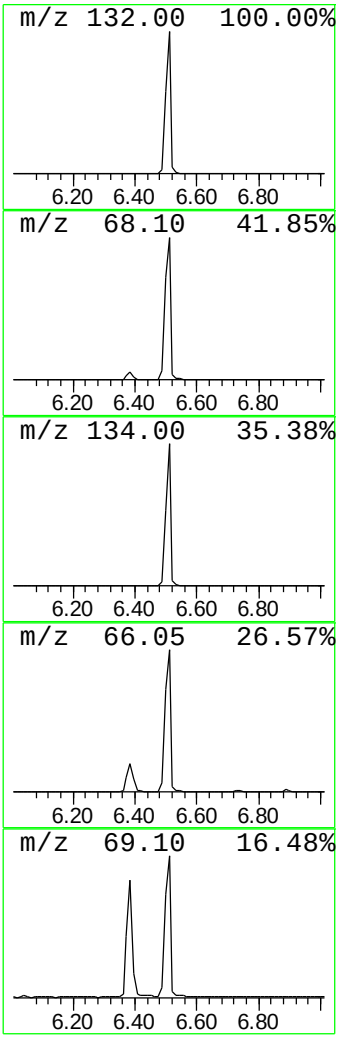
****

Peak Number 6 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	110.13 ng	5866100	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Xenon	132	Xe	007440-63-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

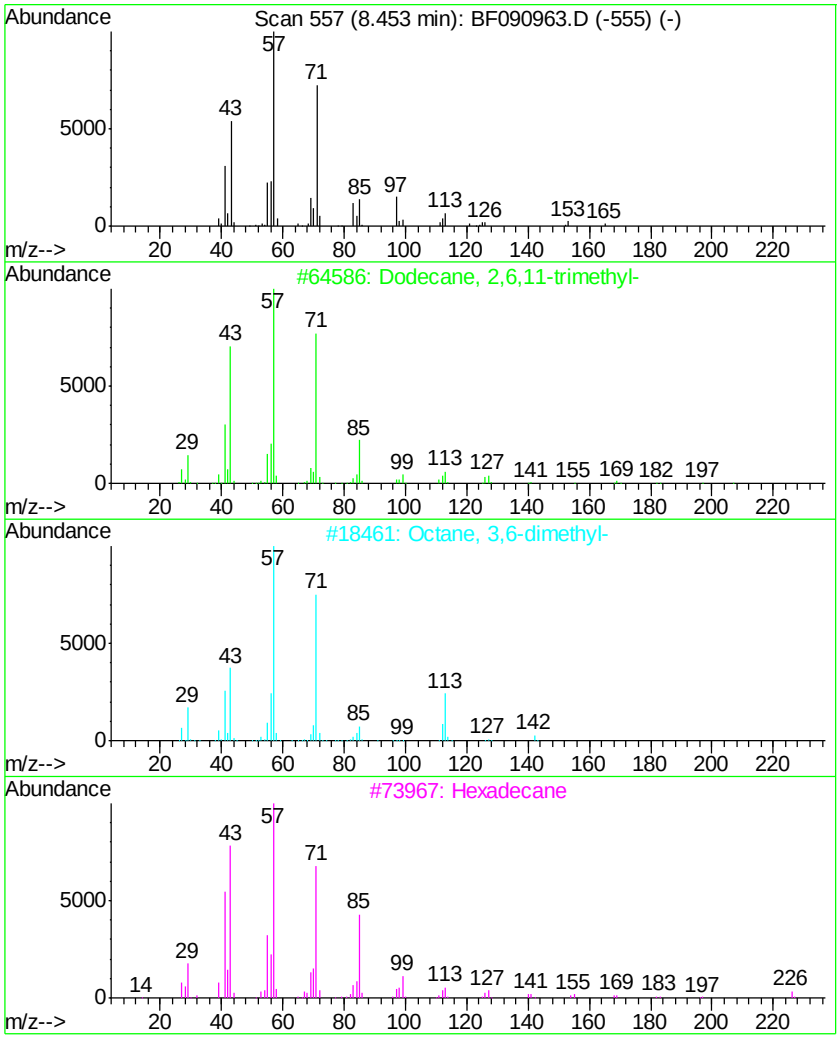
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

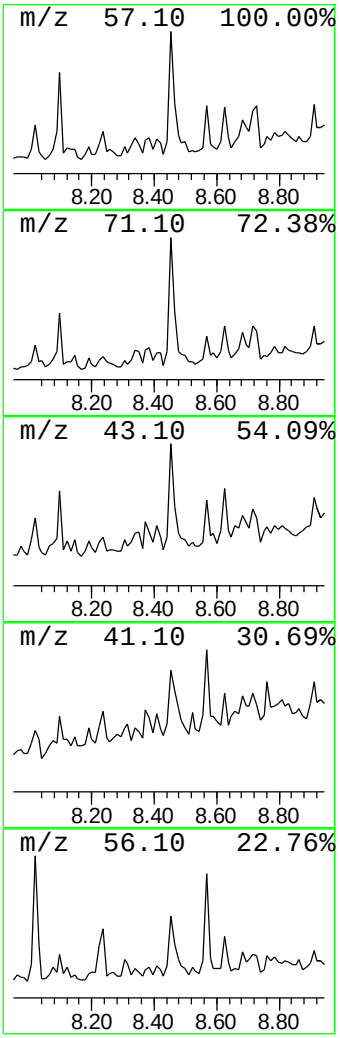
****

Peak Number 8 Dodecane, 2,6,11-trimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	2.42 ng	177040	Naphthalene-d8	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
3	Hexadecane	226	C16H34	000544-76-3	59
4	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

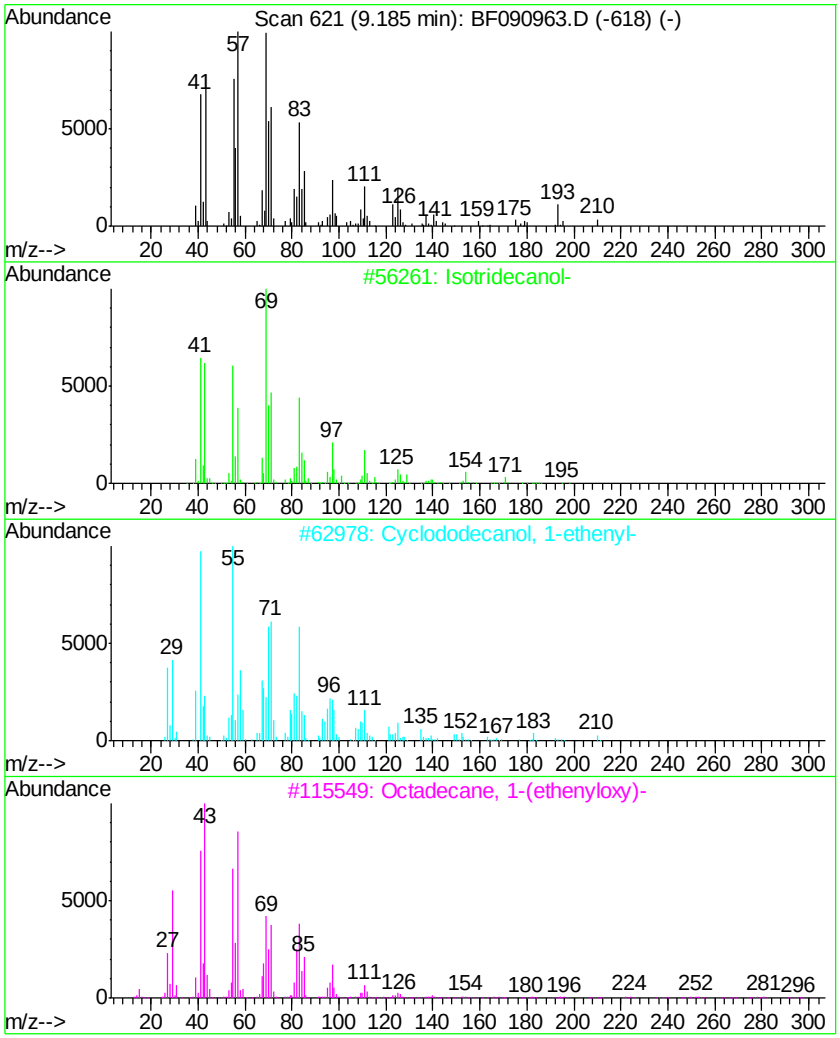
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

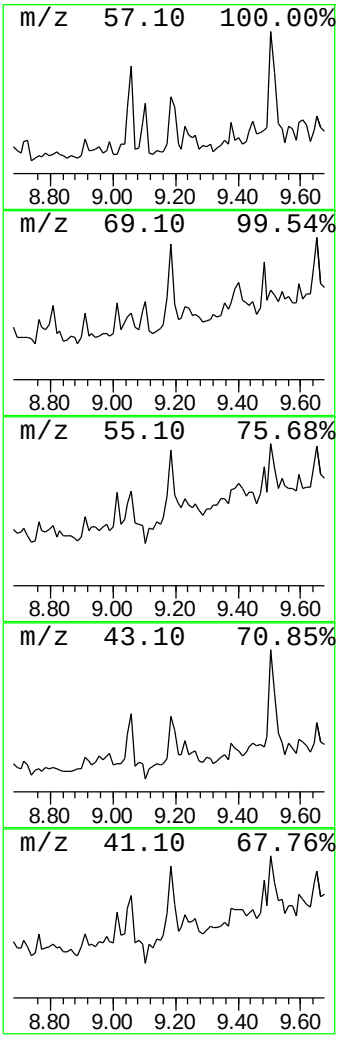
****

Peak Number 9 Isotridecanol- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.18	2.72 ng	249886	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isotridecanol-	200	C13H28O	027458-92-0	72
2	Cyclododecanol, 1-ethenyl-	210	C14H26O	006244-49-1	49
3	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	47
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	46
5	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

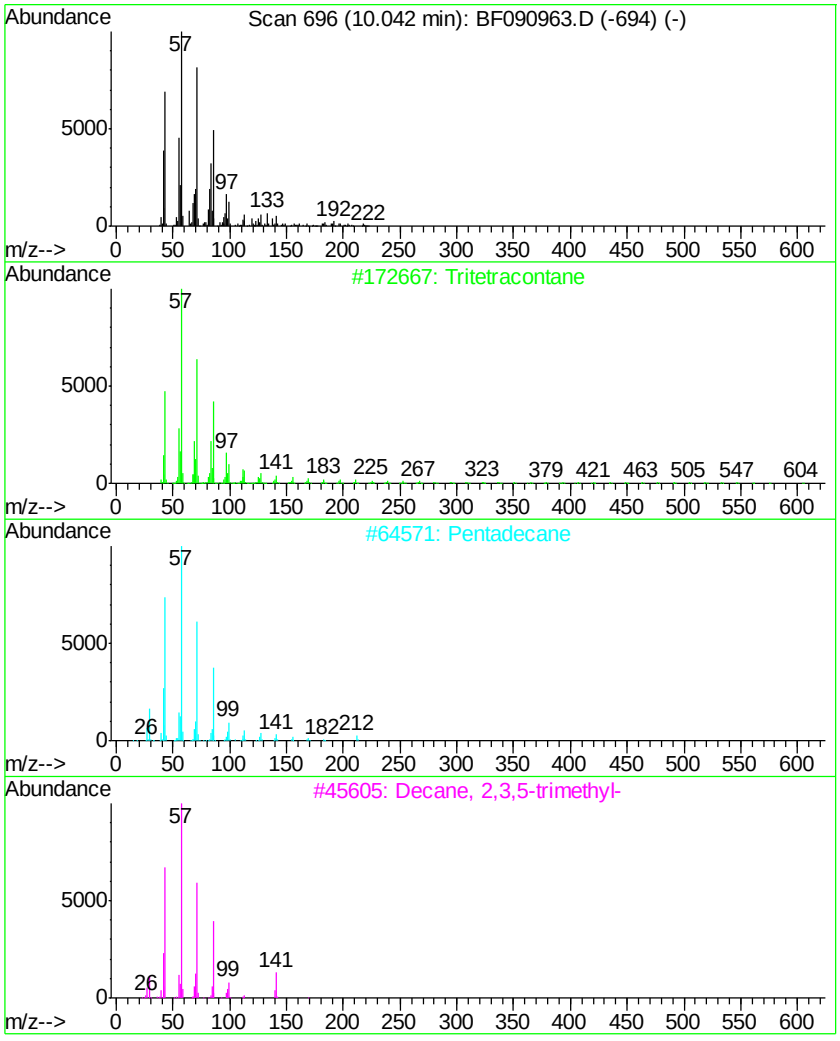
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

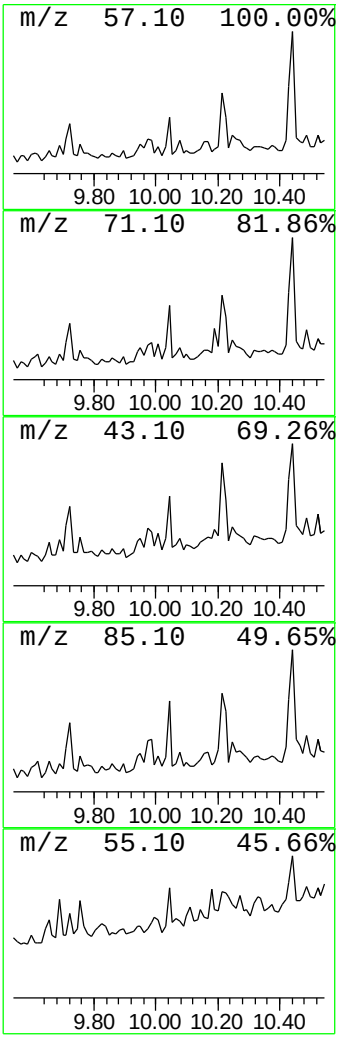
****

Peak Number 10 Tritetracontane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	2.42 ng	222418	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	80
2	Pentadecane	212	C15H32	000629-62-9	64
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	58
4	Nonadecane	268	C19H40	000629-92-5	53
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

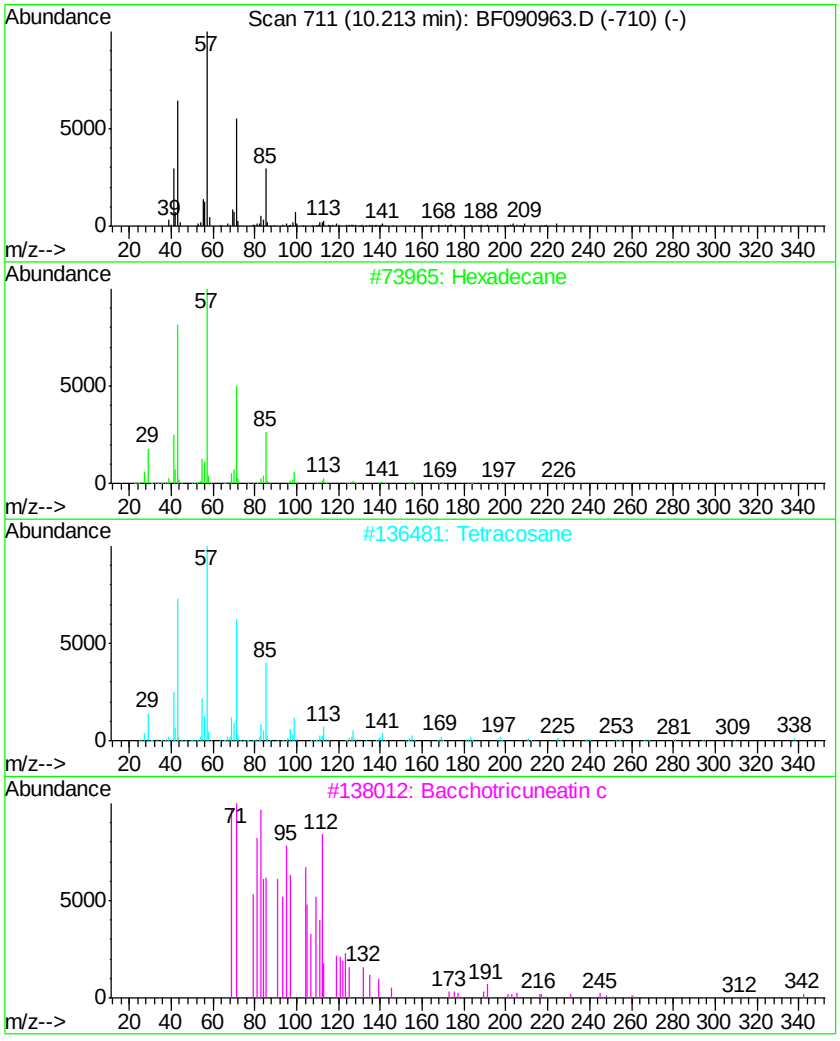
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

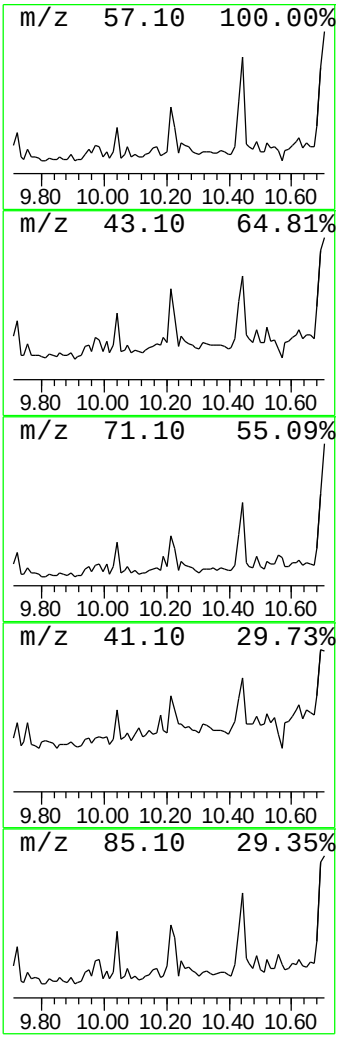
****

Peak Number 11 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.21	3.67 ng	337424	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Tetracosane	338	C24H50	000646-31-1	72
3	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
4	Heptacosane	380	C27H56	000593-49-7	64
5	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

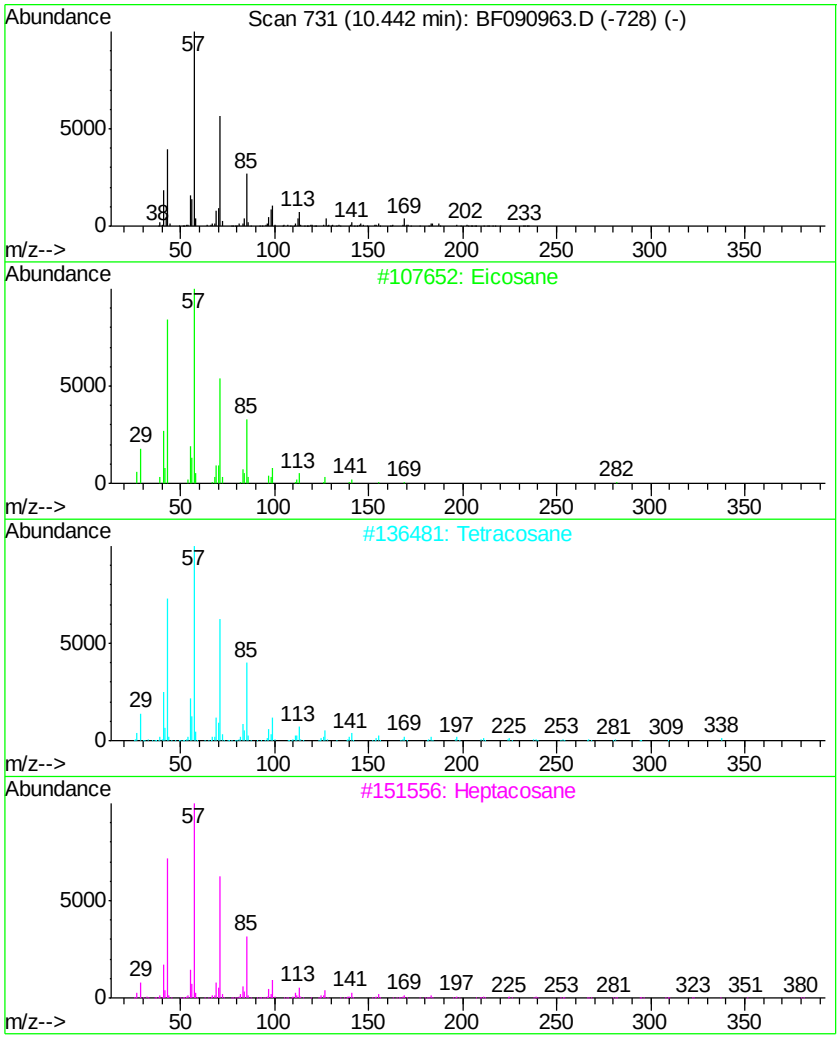
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

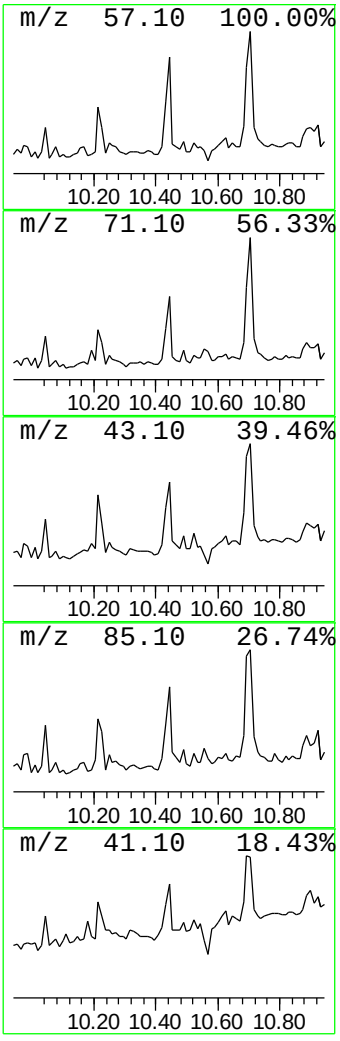
****

Peak Number 12 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	4.24 ng	389436	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Tetracosane	338	C24H50	000646-31-1	80
3	Heptacosane	380	C27H56	000593-49-7	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

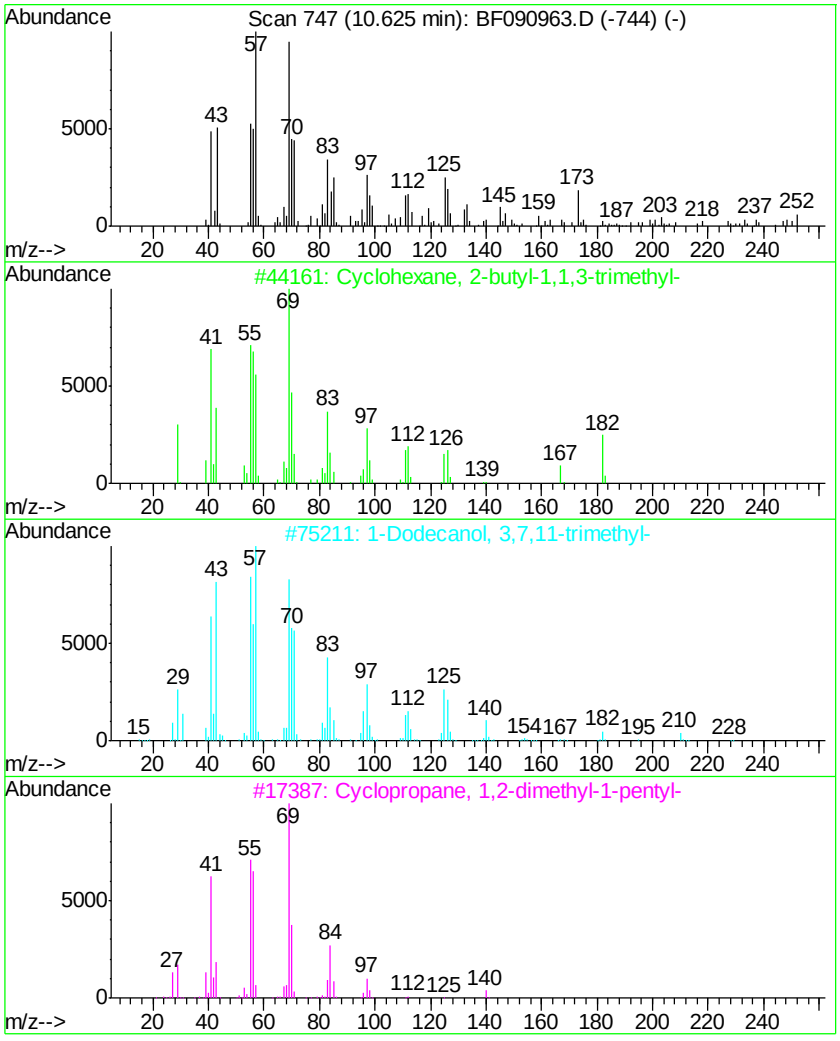
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

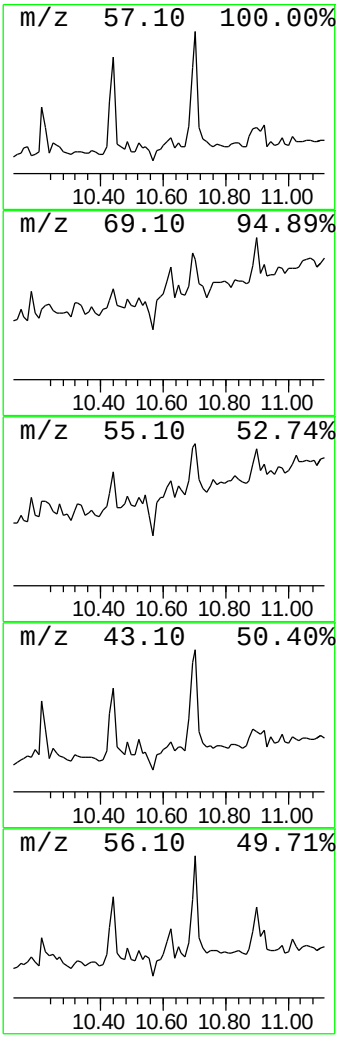
****

Peak Number 13 Cyclohexane, 2-butyl-1,1,3-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	2.83 ng	194657	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	89
2	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	86
3	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	43
4	1-Tridecene	182	C13H26	002437-56-1	42
5	2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

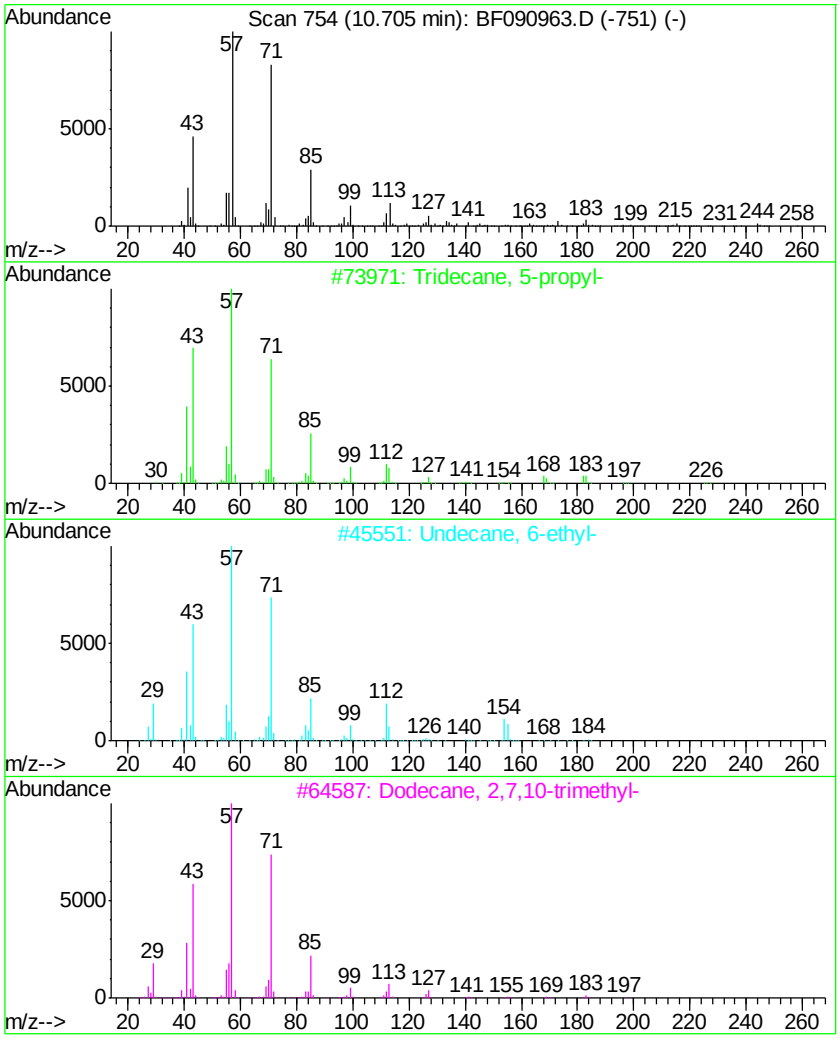
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

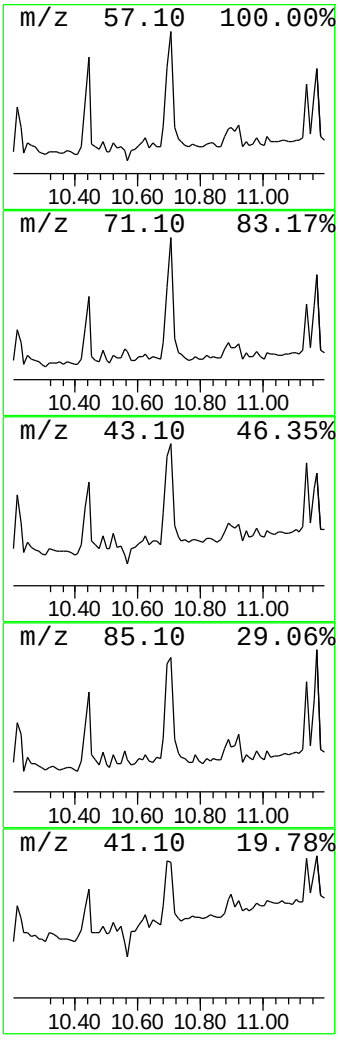
****

Peak Number 14 Tridecane, 5-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	14.72 ng	1013980	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	90
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	90
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	78
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

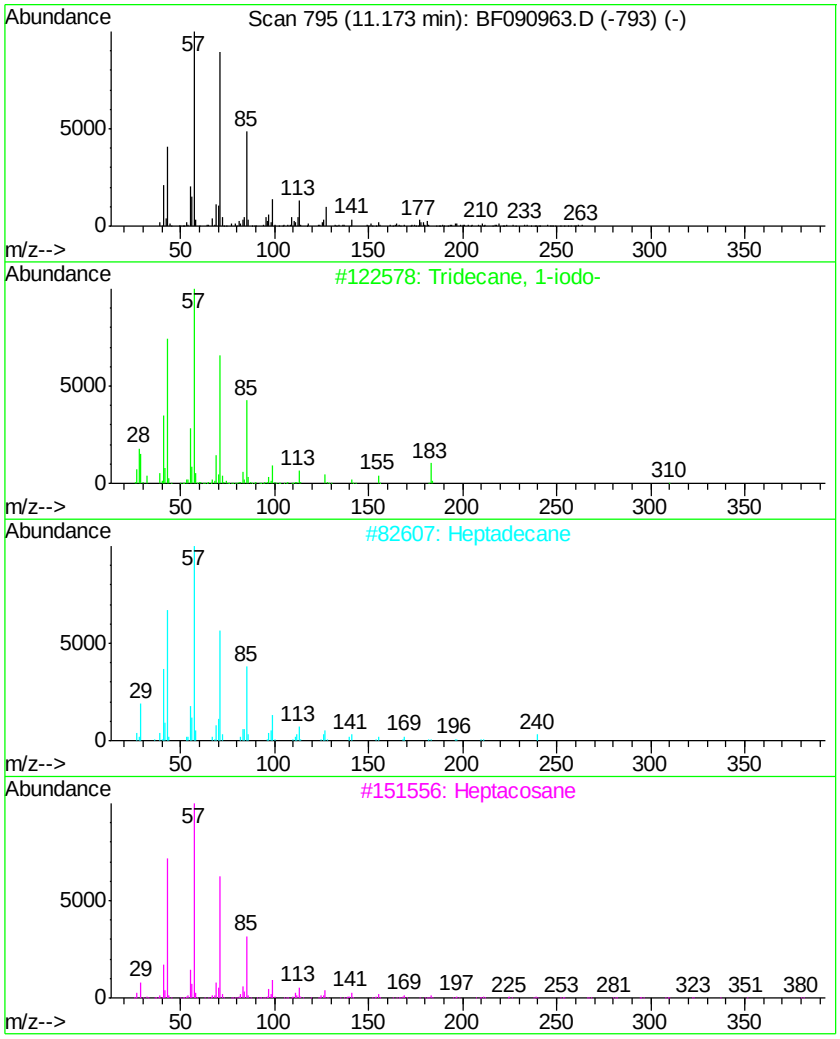
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

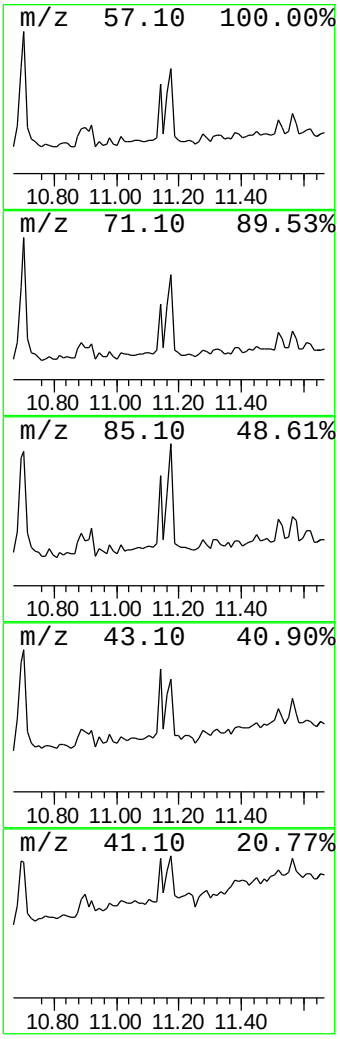
****

Peak Number 16 Tridecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	6.69 ng	460902	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
2	Heptadecane	240	C17H36	000629-78-7	64
3	Heptacosane	380	C27H56	000593-49-7	64
4	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	64
5	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

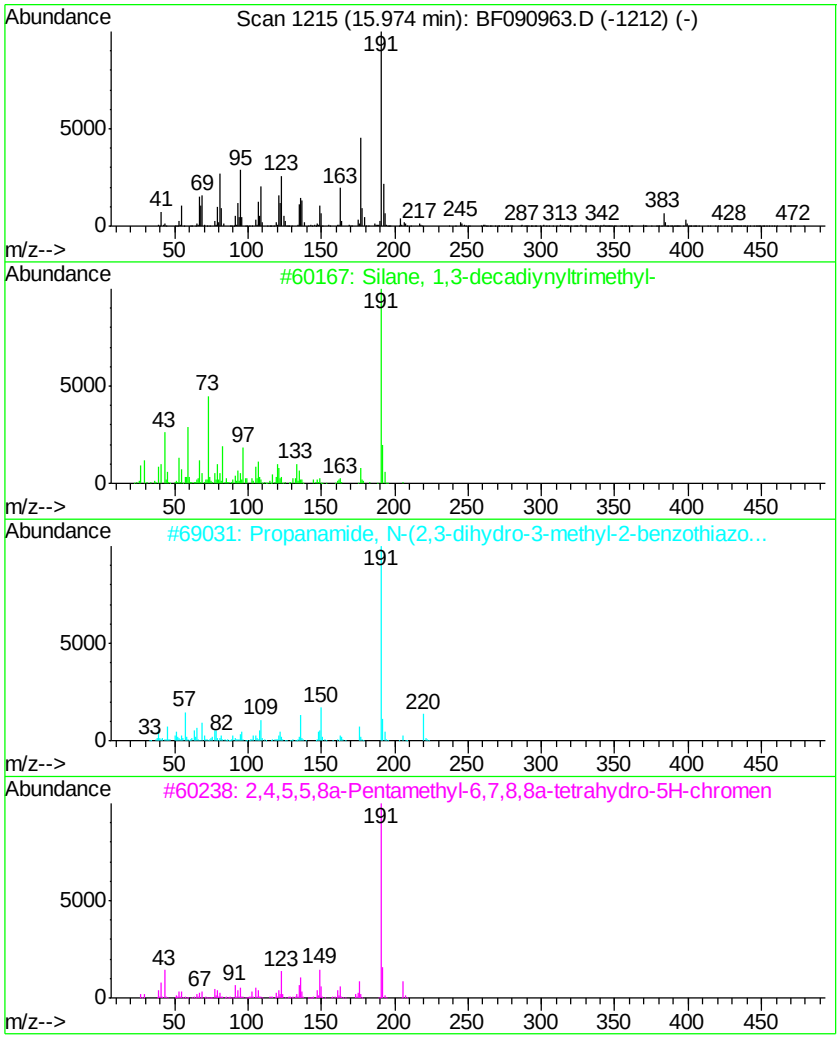
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

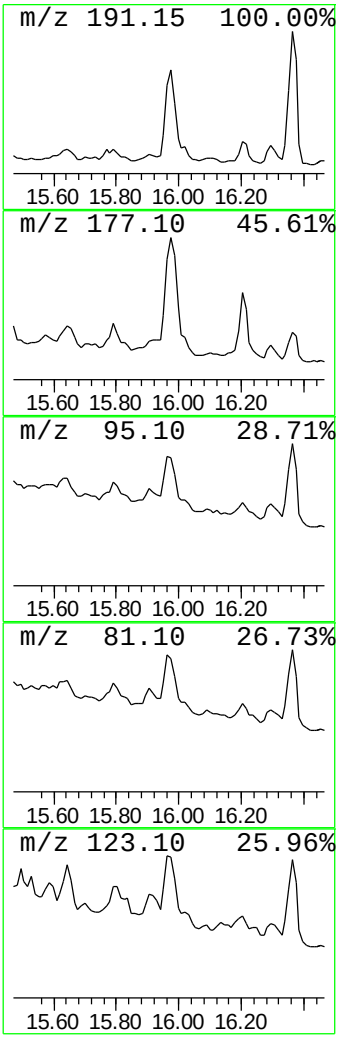
****

Peak Number 17 unknown15.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	20.00 ng	4332990	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, 1,3-decadiynyltrimethyl-	206	C13H22Si	084751-17-7	35
2	Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	35
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	32
4	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	27
5	2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

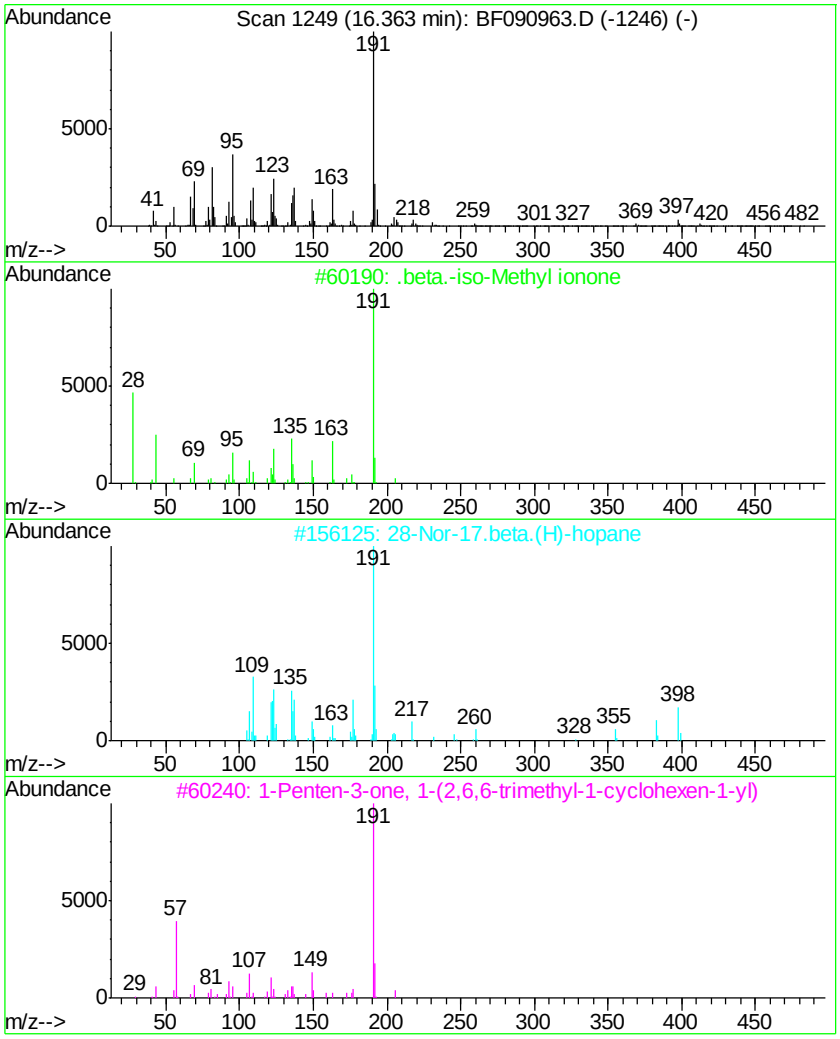
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

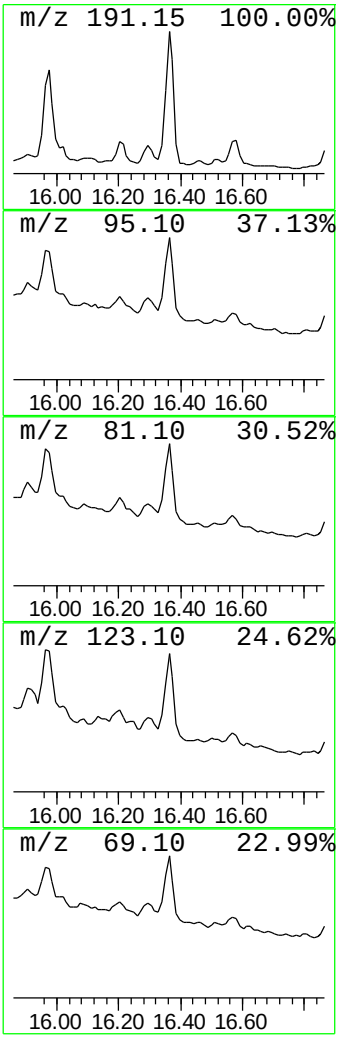
****

Peak Number 18 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	18.81 ng	4075330	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	52
2	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	50
3	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	47
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	42
5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

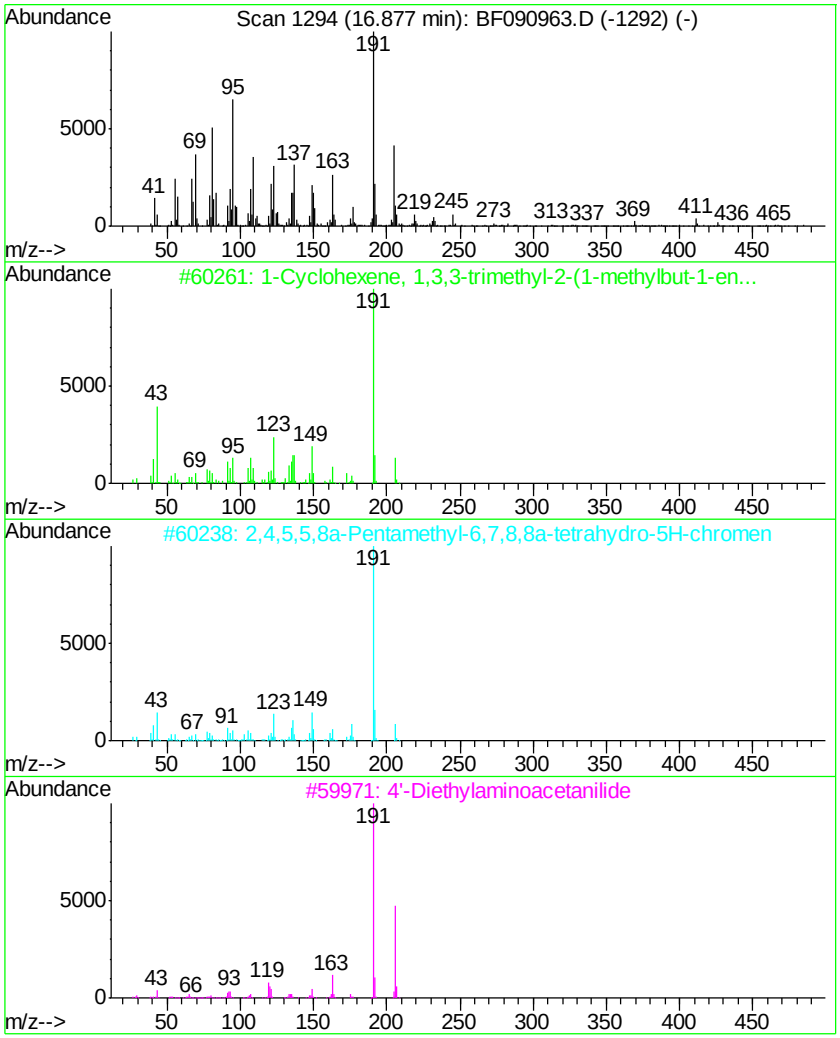
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

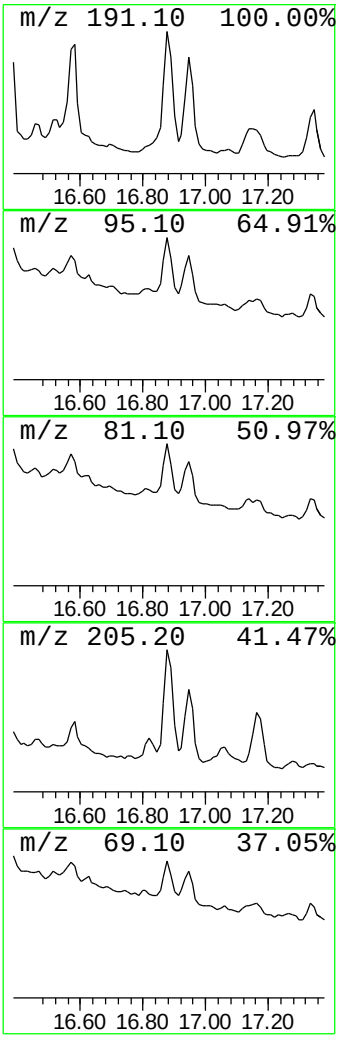
****

Peak Number 19 unknown16.88 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	5.07 ng	1099340	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	49
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43
3	4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	35
4	Silane, [4-(1,1-dimethylethyl)ph...	206	C13H22Si	018412-68-5	27
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

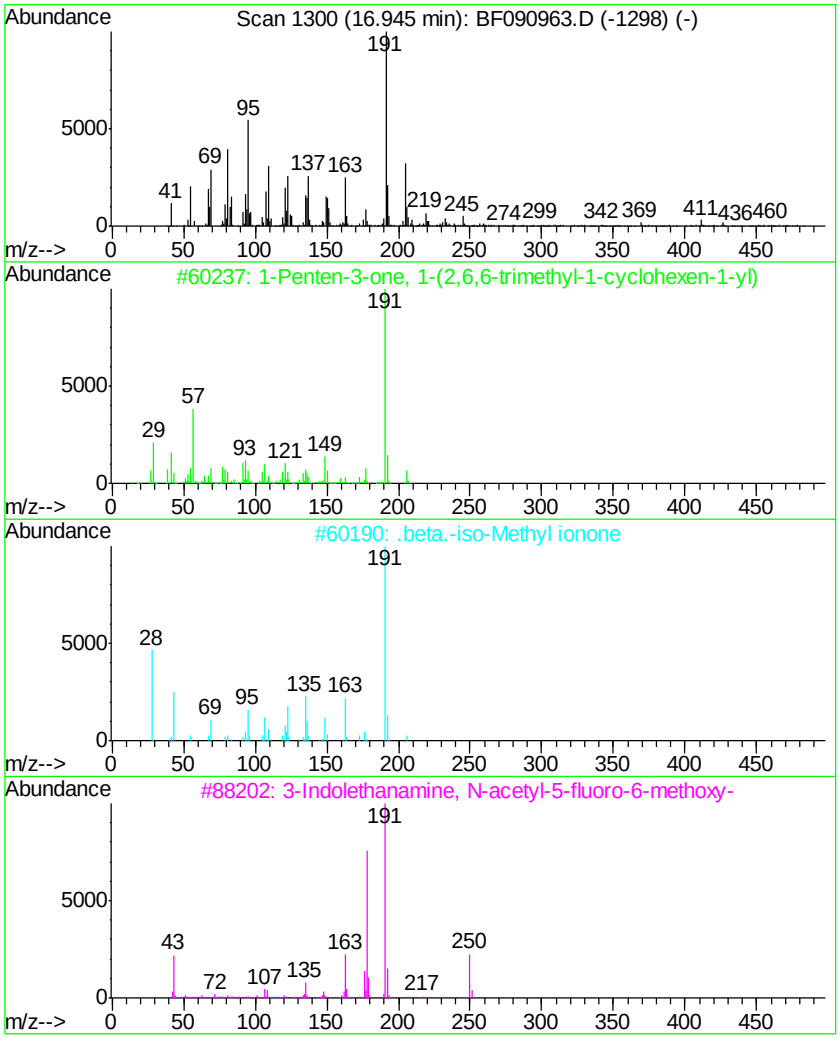
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

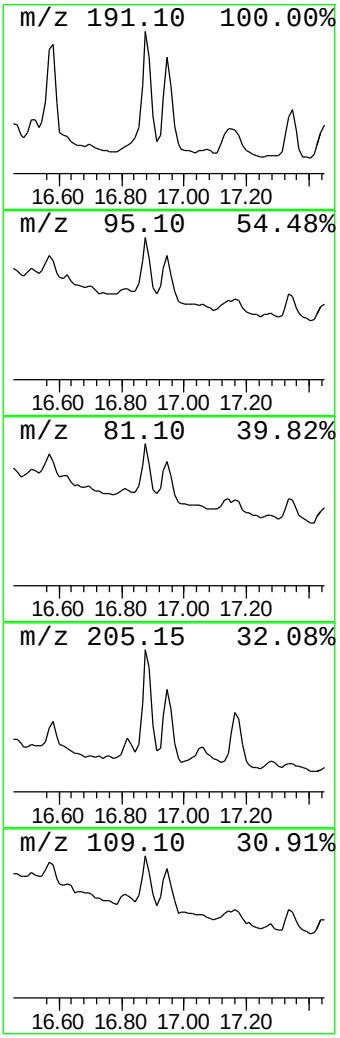
****

Peak Number 20 unknown16.95 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.95	6.63 ng	1435960	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	37
3	3-Indolethanamine, N-acetyl-5-fl...	250	C13H15FN2O2	1000116-27-1	35
4	4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	35
5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110116\
Data File : BF090963.D
Acq On : 1 Nov 2016 20:54
Operator : UM/SJ
Sample : H5491-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-78-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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
Heptane	2.14	3.5	ng	189352	1	6.74	1065350	20.0
Heptane, 3-methyl-	3.72	2.7	ng	143500	1	6.74	1065350	20.0
Octane	4.26	5.0	ng	267738	1	6.74	1065350	20.0
2-Pentanone, 4-hy...	4.90	25.3	ng	1344960	1	6.74	1065350	20.0
Nonane	5.63	2.8	ng	149222	1	6.74	1065350	20.0
unknown6.51	6.51	110.1	ng	5866100	1	6.74	1065350	20.0
Dodecane, 2,6,11-...	8.45	2.4	ng	177040	2	8.02	1465110	20.0
Isotridecanol-	9.18	2.7	ng	249886	3	9.78	1837180	20.0
Tritetracontane	10.04	2.4	ng	222418	3	9.78	1837180	20.0
Hexadecane	10.21	3.7	ng	337424	3	9.78	1837180	20.0
Eicosane	10.44	4.2	ng	389436	3	9.78	1837180	20.0
Cyclohexane, 2-bu...	10.62	2.8	ng	194657	4	11.25	1377360	20.0
Tridecane, 5-propyl-	10.70	14.7	ng	1013980	4	11.25	1377360	20.0
Tridecane, 1-iodo-	11.17	6.7	ng	460902	4	11.25	1377360	20.0
unknown15.97	15.97	20.0	ng	4332990	6	15.32	4332990	20.0
.beta.-iso-Methyl...	16.36	18.8	ng	4075330	6	15.32	4332990	20.0
unknown16.88	16.88	5.1	ng	1099340	6	15.32	4332990	20.0
unknown16.95	16.95	6.6	ng	1435960	6	15.32	4332990	20.0