LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

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-BF122116.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	1.913	9	11	16	rVB3	86999	195517	2.76%	0.257%
2	2.084	24	26	31	rVB3	66942	131868	1.86%	0.174%
3	2.278	39	43	49	rVB3	65430	248332	3.51%	0.327%
4	2.598	66	71	80	rVV2	105551	276560	3.91%	0.364%
5	2.758	80	85	88	rVV2	111248	267914	3.78%	0.353%
6	2.815	88	90	95	rVV2	52905	103685	1.46%	0.137%
7	2.953	99	102	106	rVV2	44829	118344	1.67%	0.156%
8	3.056	106	111	114	rVV	98211	233535	3.30%	0.308%
9	3.136	114	118	122	rVV	86074	187124	2.64%	0.246%
10	3.250	122	128	138	rVB4	35564	132251	1.87%	0.174%
11	3.410	138	142	146	rBV2	32803	72860	1.03%	0.096%
12	3.536	146	153	160	rVB5	103390	365365	5.16%	0.481%
13	3.718	165	169	173	rBV2	195792	475655	6.72%	0.626%
14	3.810	173	177	179	rBV2	99976	233313	3.29%	0.307%
15	3.970	186	191	198	rVB	514542	1135945	16.04%	1.496%
16	4.118	198	204	211	rBV2	1001068	1944468	27.46%	2.561%
17	4.221	211	213	216	rVB2	57288	89600	1.27%	0.118%
18	4.290	216	219	223	rVB2	95916	206982	2.92%	0.273%
19	4.404	223	229	231	rBV	419095	755733	10.67%	0.995%
20	4.439	231	232	235	rVB	375359	401393	5.67%	0.529%
21	4.484	235	236	238	rBV	112321	167456	2.36%	0.221%
22	4.519	238	239	243	rVB	181043	241714	3.41%	0.318%
23	4.576	243	244	247	rVB	69346	95076	1.34%	0.125%
24	4.679	247	253	256	rBV	651620	1353424	19.11%	1.782%
25	4.724	256	257	260	rVB	222175	211557	2.99%	0.279%
26	4.873	268	270	273	rVB2	91997	145964	2.06%	0.192%
27	4.930	273	275	276	rBV	190414	223825	3.16%	0.295%
28	4.953	276	277	280	rVB	161393	214614	3.03%	0.283%
29	5.021	280	283	285	rBV3	89119	171521	2.42%	0.226%
30	5.067	285	287	289	rBV	555564	624695	8.82%	0.823%
31	5.101	289	290	293	rVB	316373	335372	4.74%	0.442%
32	5.147	293	294	298	rBV	2232642	3283939	46.37%	4.324%
33	5.273	303	305	308	rBV2	225945	316354	4.47%	0.417%
34	5.376	311	314	316	rBV2	202646	328465	4.64%	0.433%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	5.410	316	317	318	rVB	115957	79547	1.12%	0.105%
36	5.444	318	320	323	rVB3	60055	102456	1.45%	0.135%
37	5.524	323	327	331	rBV3	267411	654905	9.25%	0.862%
38	5.593	331	333	335	rVB2	104996	163396	2.31%	0.215%
39	5.627	335	336	338	rVB	59371	73017	1.03%	0.096%
40	5.684	338	341	346	rBV2	451117	1302808	18.40%	1.716%
41	5.787	348	350	354	rVB3	133130	232702	3.29%	0.306%
42	5.856	354	356	357	rBV2	159868	255720	3.61%	0.337%
43	5.890	357	359	361	rVB	181931	195850	2.77%	0.258%
44	5.959	361	365	368	rVB3	372549	687031	9.70%	0.905%
45	6.016	368	370	372	rVB3	86057	99426	1.40%	0.131%
46	6.073	372	375	377	rBV2	173991	346880	4.90%	0.457%
47	6.222	386	388	395	rBV	1350338	2006334	28.33%	2.642%
48	6.336	395	398	400	rBV	5452526	5669869	80.06%	7.466%
49	6.439	406	407	410	rVB2	104129	99679	1.41%	0.131%
50	6.519	410	414	416	rBV2	443273	744892	10.52%	0.981%
51	6.564	416	418	420	rVV	1000406	1290771	18.23%	1.700%
52	6.599	420	421	424	rVB3	78389	100360	1.42%	0.132%
53	6.644	424	425	426	rBV	68899	90736	1.28%	0.119%
54	6.679	426	428	429	rVB	350997	281657	3.98%	0.371%
55	6.713	429	431	434	rBV	3977455	4910234	69.33%	6.466%
56	6.827	439	441	443	rVB3	68193	97109	1.37%	0.128%
57	6.884	445	446	450	rBV	555291	709984	10.03%	0.935%
58	6.953	450	452	454	rBV2	142107	150414	2.12%	0.198%
59	6.999	454	456	458	rBV3	43226	81440	1.15%	0.107%
60	7.033	458	459	463	rVB2	73380	87052	1.23%	0.115%
61	7.136	465	468	472	rVV	4408469	4912181	69.36%	6.469%
62	7.216	472	475	476	rVV3	134152	239471	3.38%	0.315%
63	7.262	476	479	483	rVV2	290908	424326	5.99%	0.559%
64	7.330	483	485	488	rVB3	197012	333901	4.71%	0.440%
65	7.422	490	493	494	rBV2	376671	537099	7.58%	0.707%
66	7.502	497	500	501	rBV	374556	337630	4.77%	0.445%
67	7.536	501	503	505	rVB2	460201	538752	7.61%	0.709%
68	7.593	505	508	510	rBV2	197455	277729	3.92%	0.366%
69	7.662	510	514	516	rBV2	143606	358269	5.06%	0.472%
70	7.787	523	525	528	rBV2	126499	186638	2.64%	0.246%
71	7.845	528	530	534	rVV2	1455918	2585619	36.51%	3.405%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	7.902	534	535	541	rVB3	106082	205194	2.90%	0.270%
73	8.050	546	548	550	rBV3	95750	177399	2.50%	0.234%
74	8.096	550	552	556	rVV3	92402	189260	2.67%	0.249%
75	8.519	587	589	590	rVB	102362	115583	1.63%	0.152%
76	8.542	590	591	595	rVB4	54817	74231	1.05%	0.098%
77	8.645	598	600	603	rBV2	59598	85558	1.21%	0.113%
78	8.736	606	608	610	rBV3	88775	103945	1.47%	0.137%
79	8.828	612	616	619	rVB4	50180	76858	1.09%	0.101%
80	8.930	622	625	627	rBV	6791726	7049322	99.54%	9.283%
81	9.593	680	683	685	rBV	2514403	2326036	32.84%	3.063%
82	9.833	702	704	706	rBV3	72564	98434	1.39%	0.130%
83	9.868	706	707	710	rVB2	69192	84947	1.20%	0.112%
84	10.382	749	752	755	rBV2	3573450	4658065	65.77%	6.134%
85	10.771	784	786	791	rVB2	58815	73425	1.04%	0.097%
86	11.068	810	812	815	rBV	2281305	2141261	30.24%	2.820%
87	11.628	858	861	872	rBV2	256187	418869	5.91%	0.552%
88	12.405	927	929	932	rBV	329152	394076	5.56%	0.519%
89	12.656	948	951	954	rBV	5714146	7082036	100.00%	9.326%
90	13.697	1039	1042	1044	rBV	2073411	2033453	28.71%	2.678%
91	15.045	1157	1160	1162	rBV	1262162	1434085	20.25%	1.888%
92	15.080	1162	1163	1168	rVB	86511	136363	1.93%	0.180%
93	15.445	1192	1195	1198	rBV	79582	123127	1.74%	0.162%
94	15.845	1227	1230	1236	rVB	73289	147469	2.08%	0.194%
95	16.325	1269	1272	1277	rBV	44292	78637	1.11%	0.104%
96	16.885	1316	1321	1328	rVB2	31903	94821	1.34%	0.125%

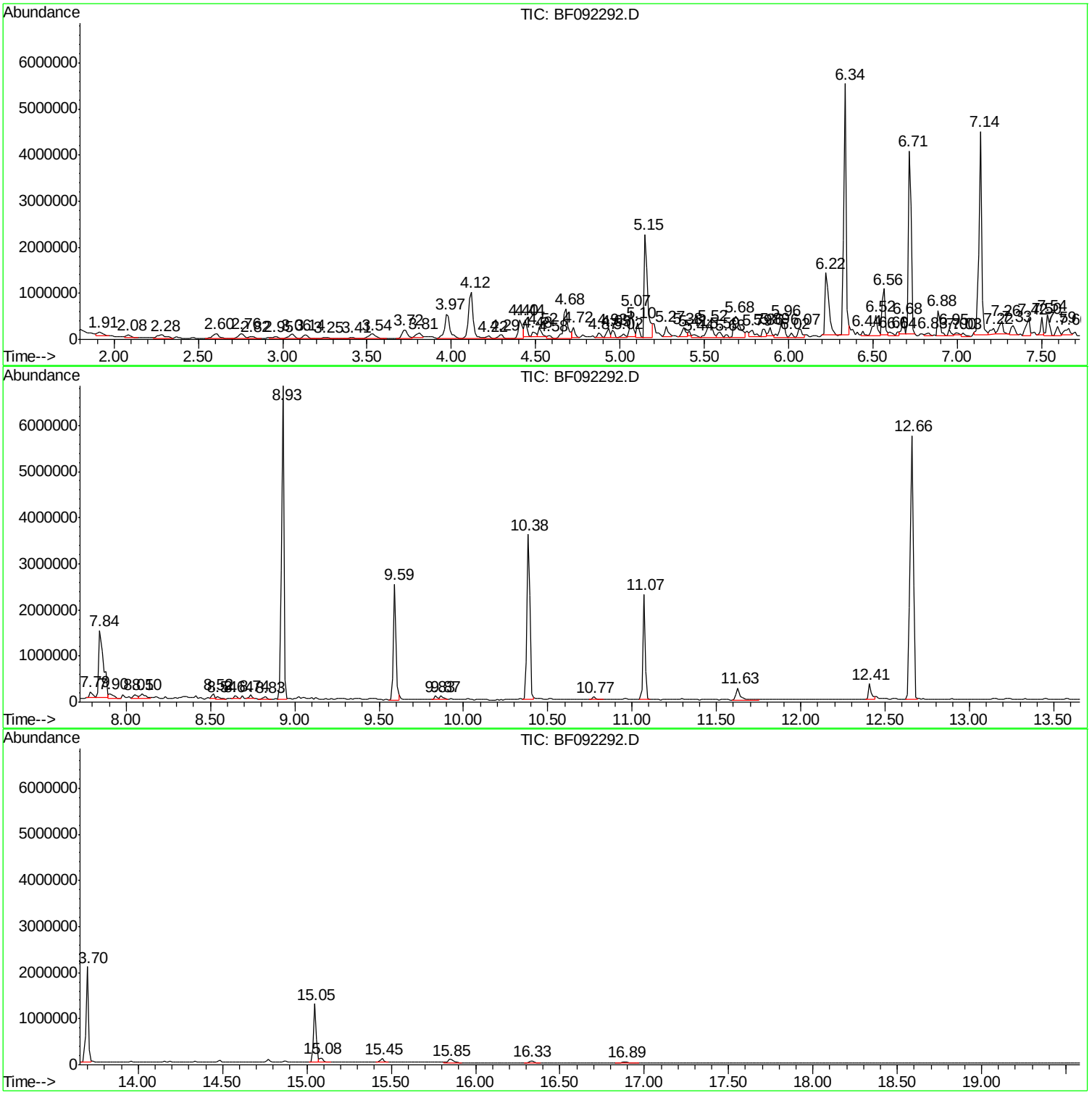
Sum of corrected areas: 75938758

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

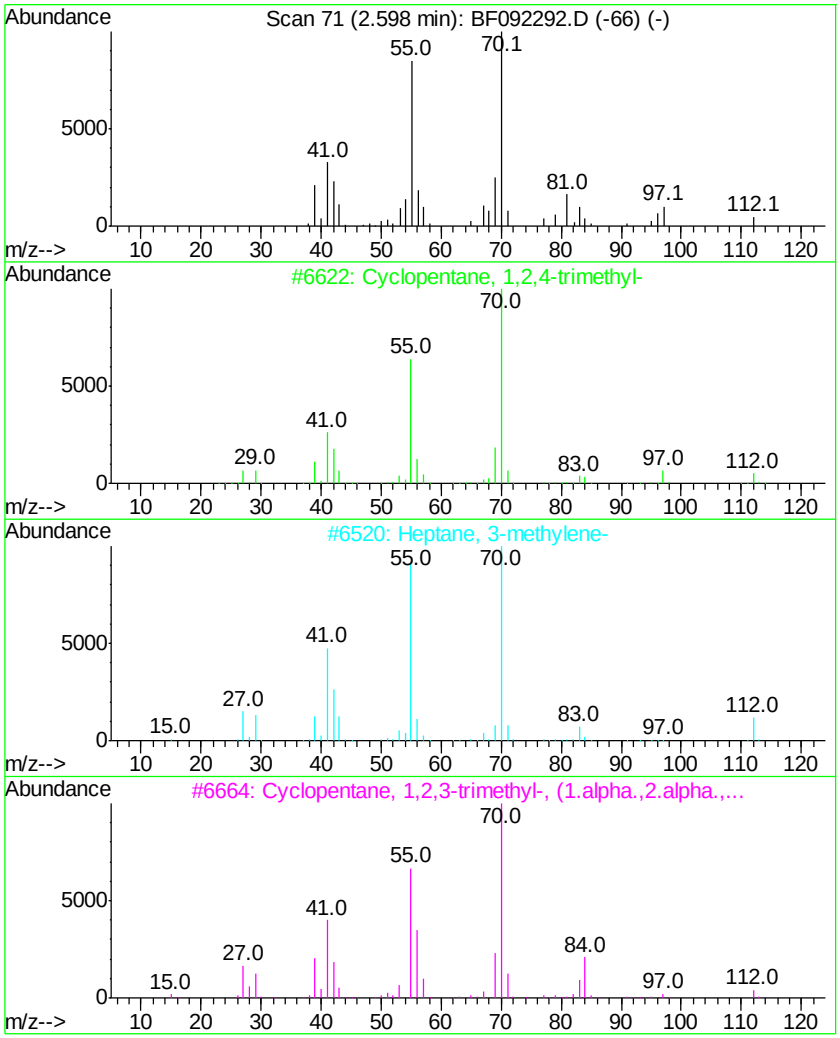
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

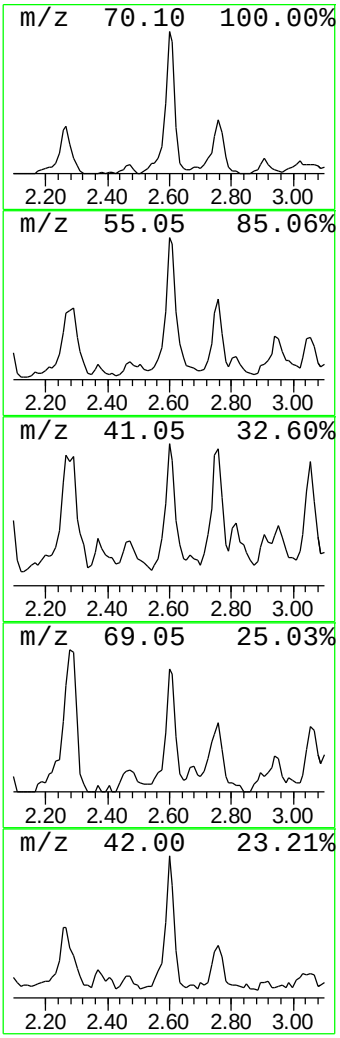
****

Peak Number 1 Cyclopentane, 1,2,4-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.60	4.29 ng	276560	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	80
2	Heptane, 3-methylene-	112	C8H16	001632-16-2	72
3	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	72
4	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	64
5	Nonane, 3-methylene-	140	C10H20	051655-64-2	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

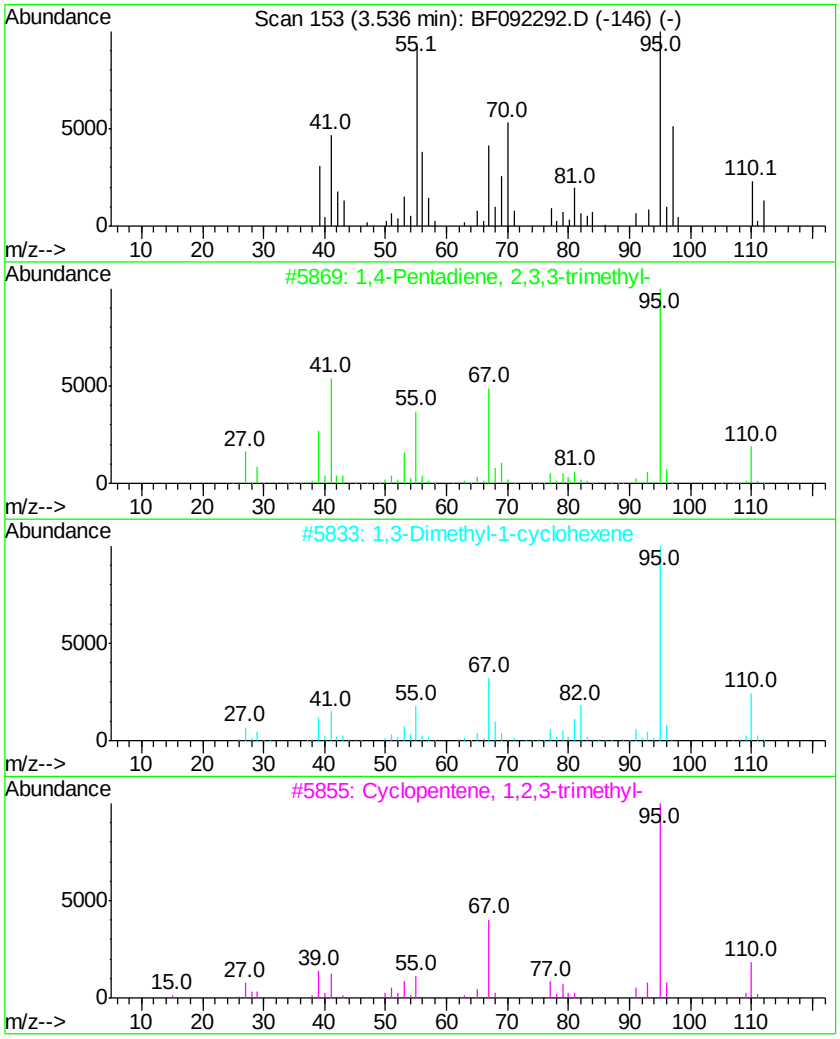
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

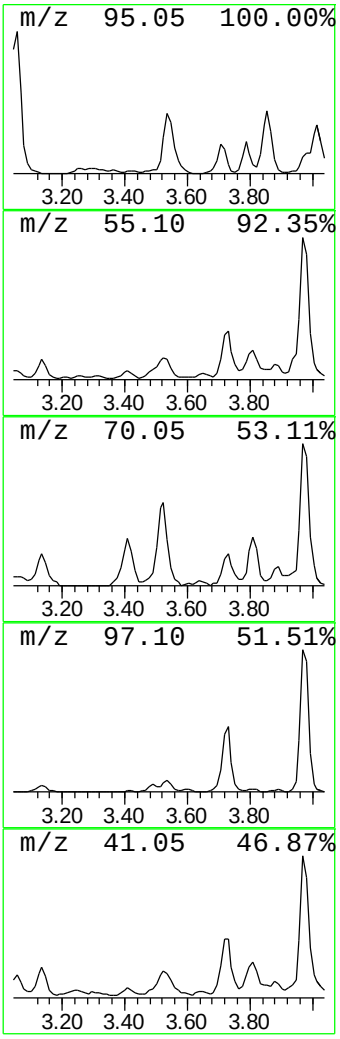
****

Peak Number 2 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	5.66 ng	365365	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	50
2	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	50
3	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	50
4	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	50
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

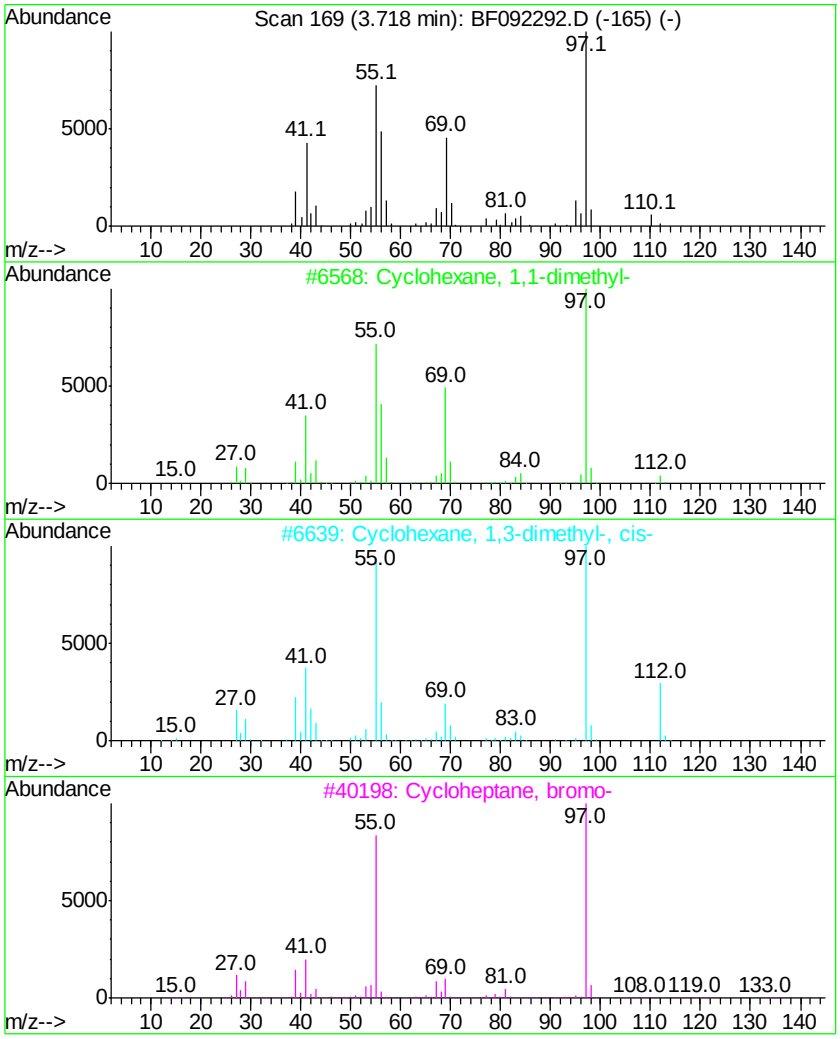
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

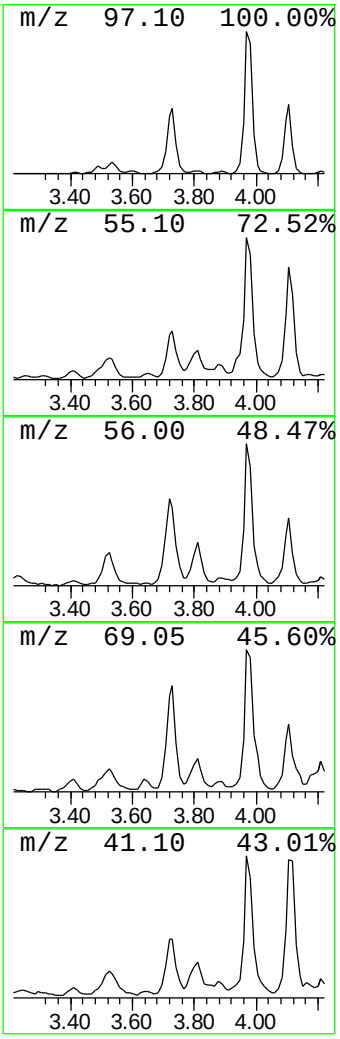
****

Peak Number 3 Cyclohexane, 1,1-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	7.37 ng	475655	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	80
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	59
3	Cycloheptane, bromo-	176	C7H13Br	002404-35-5	47
4	3-Penten-1-ol, 2,2,4-trimethyl-	128	C8H16O	005842-53-5	47
5	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	45





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

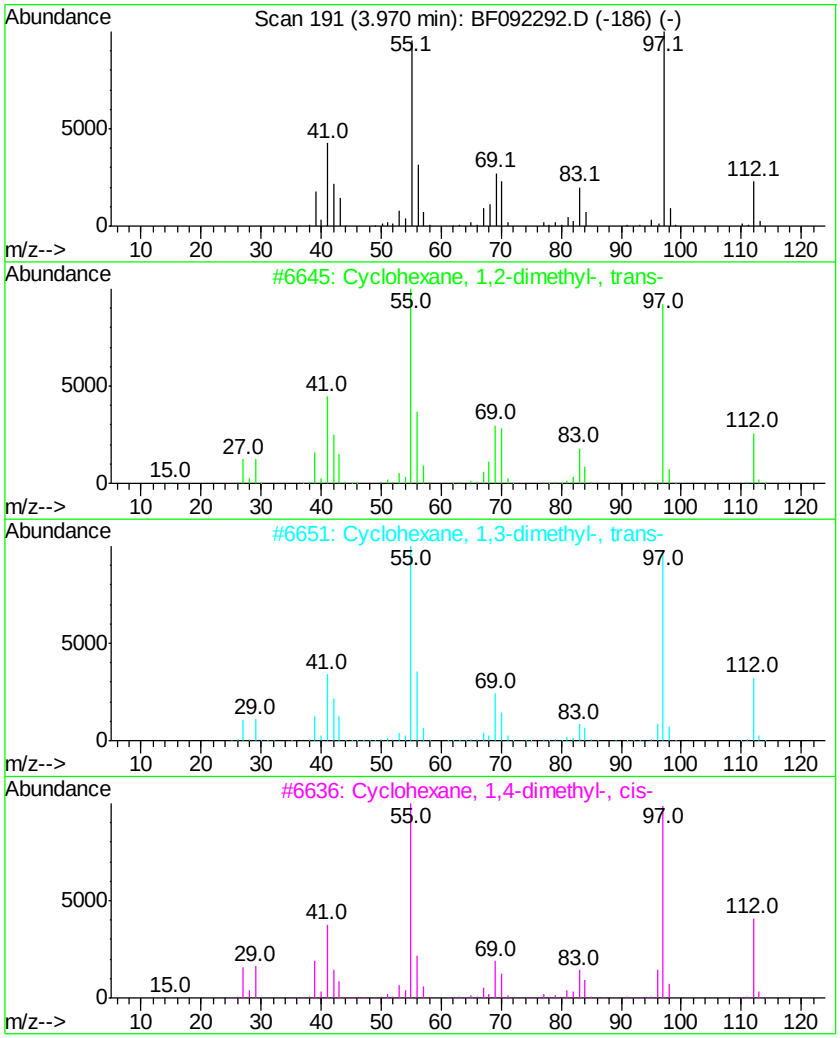
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

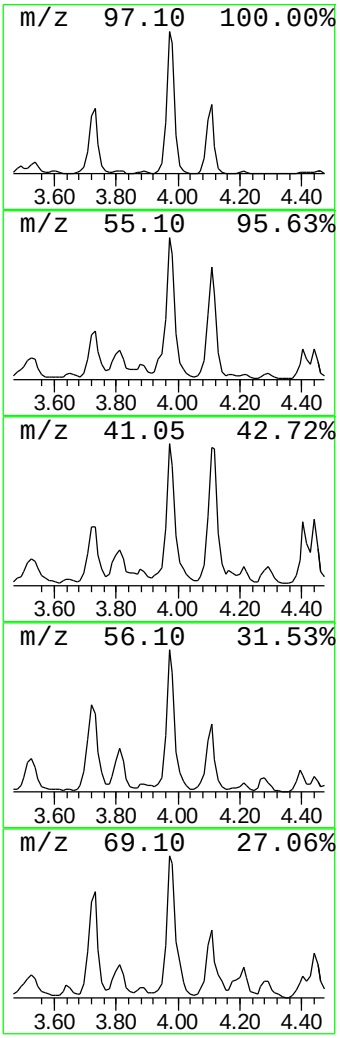
****

Peak Number 4 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.97	17.60 ng	1135950	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	96
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	87
3	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	83
4	1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	76
5	Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

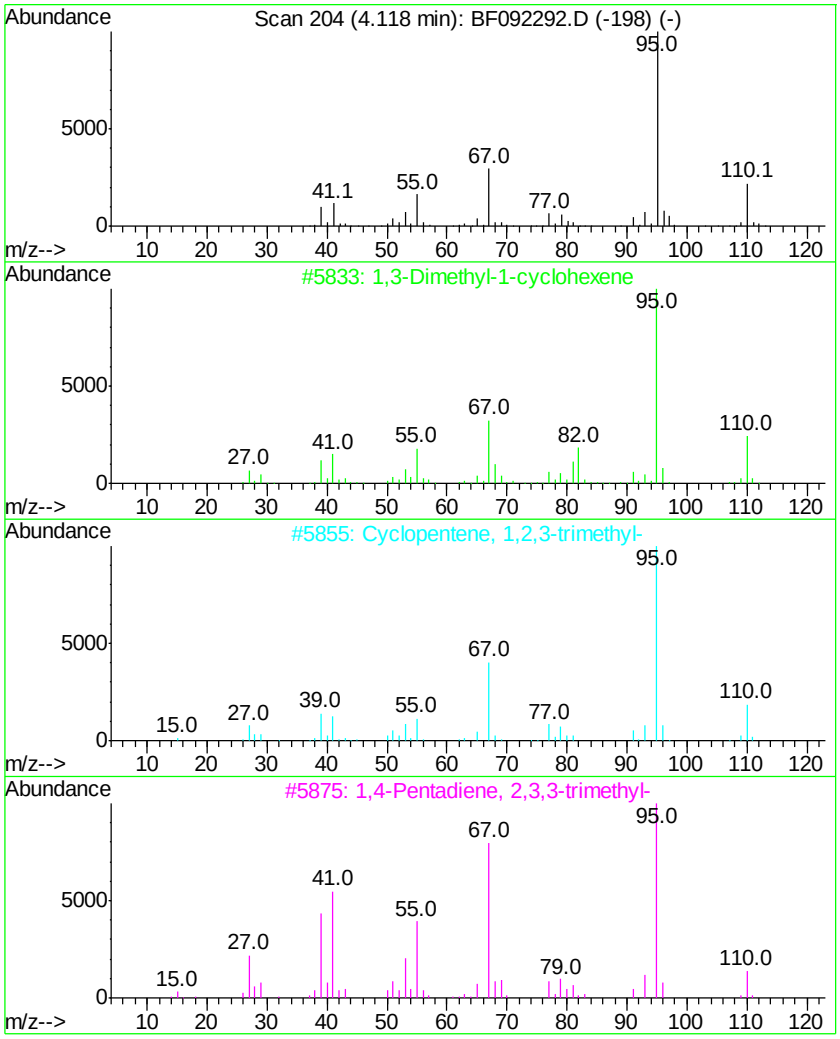
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

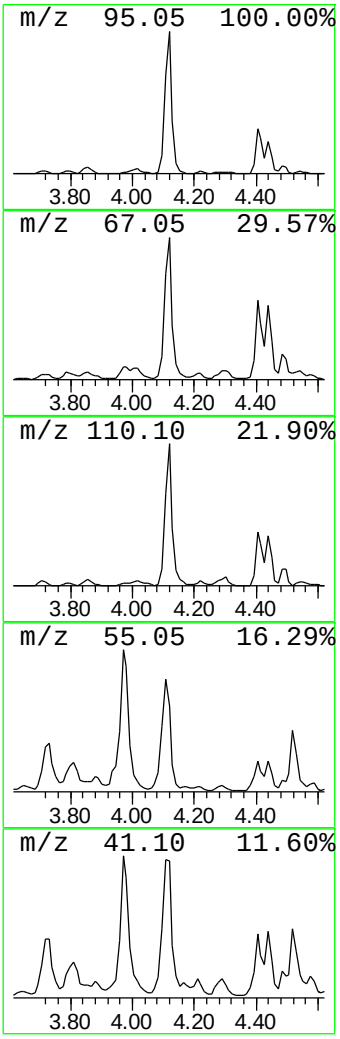
****

Peak Number 5 1,3-Dimethyl-1-cyclohexene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	30.13 ng	1944470	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	91
2	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	90
3	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	87
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	78
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

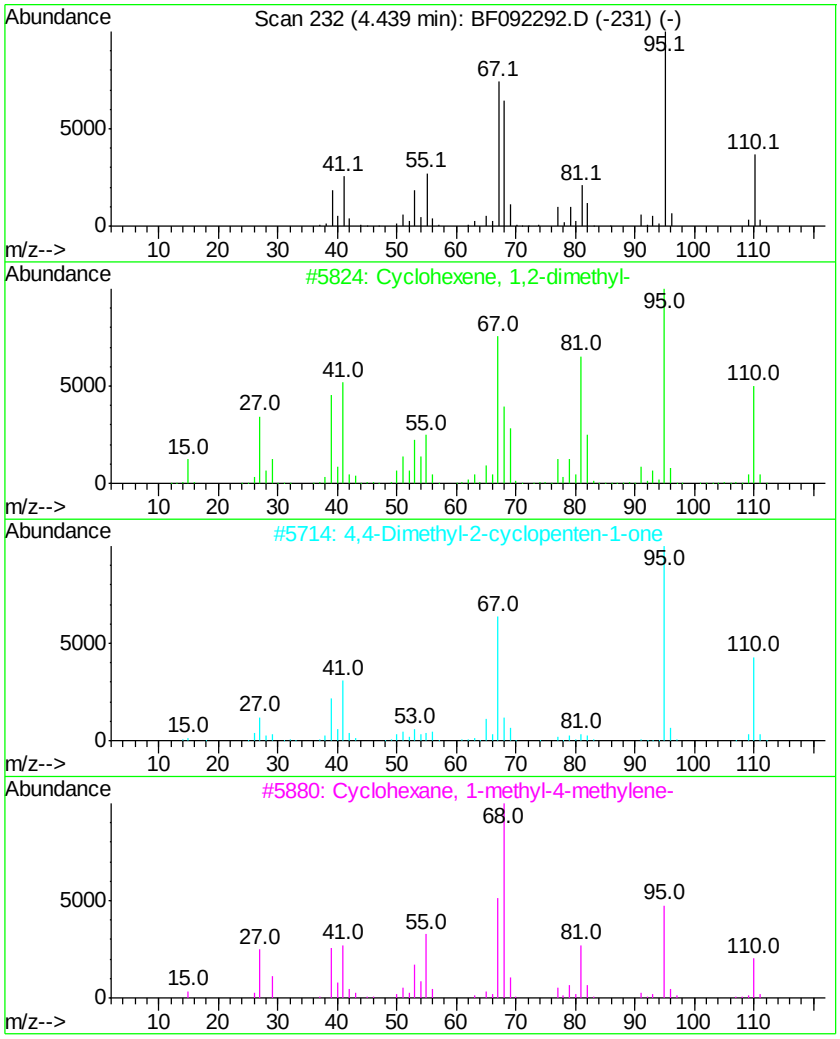
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

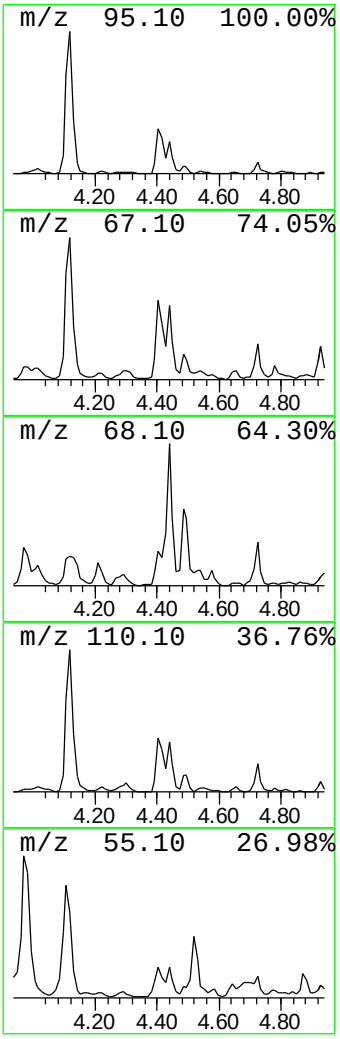
****

Peak Number 7 Cyclohexene, 1,2-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	6.22 ng	401393	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	83
2	4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	76
3	Cyclohexane, 1-methyl-4-methylene-	110	C8H14	002808-80-2	68
4	1-Methylcycloheptene	110	C8H14	055308-20-8	68
5	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

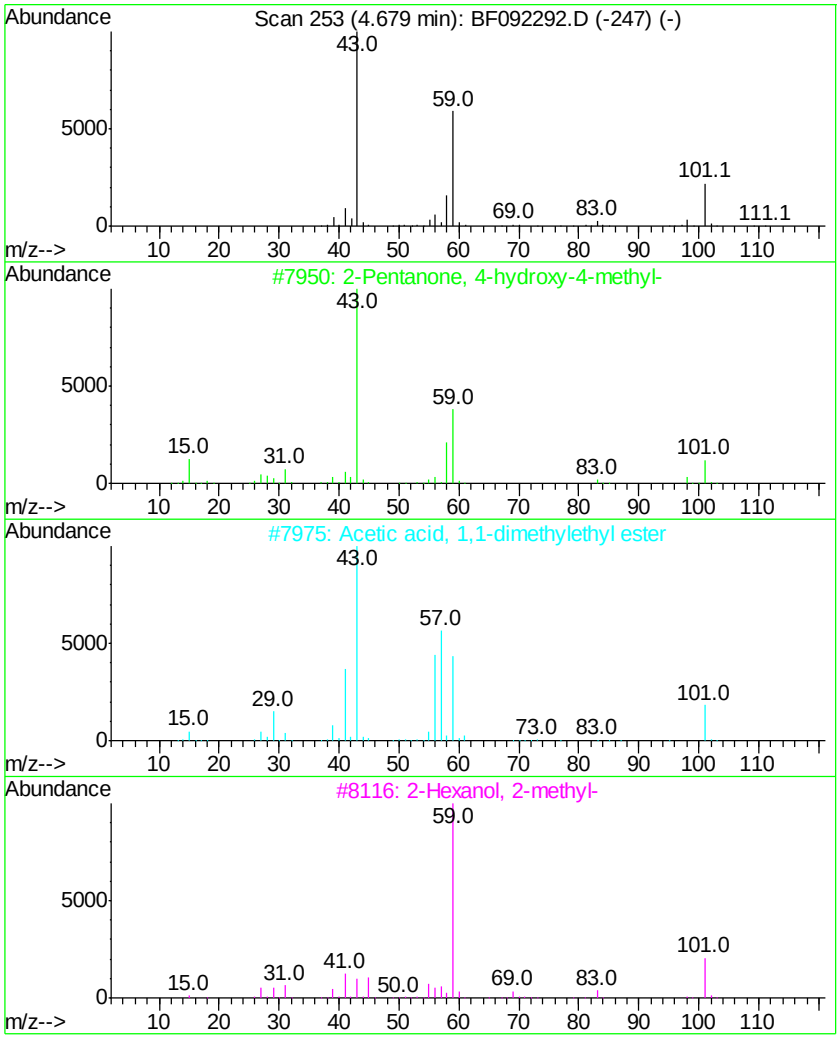
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

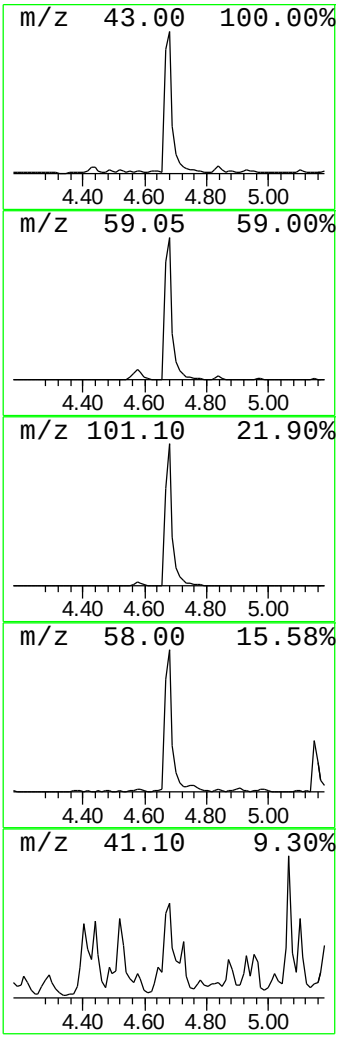
****

Peak Number 8 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	20.97 ng	1353420	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

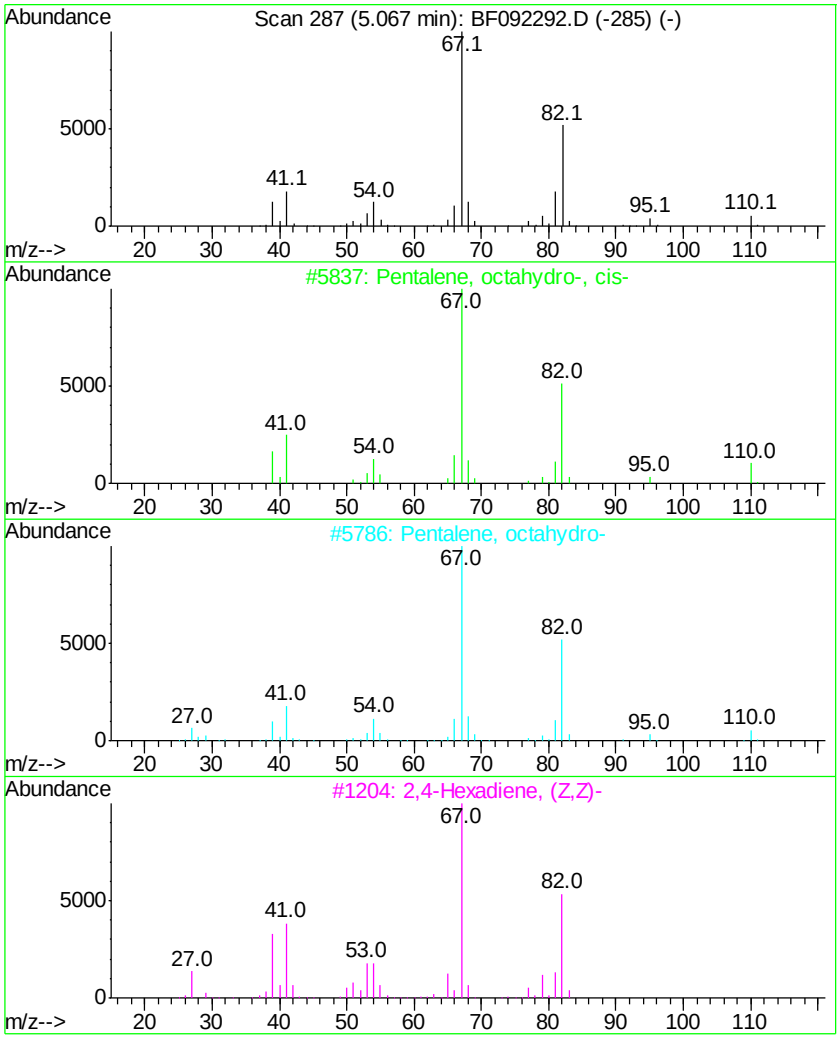
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

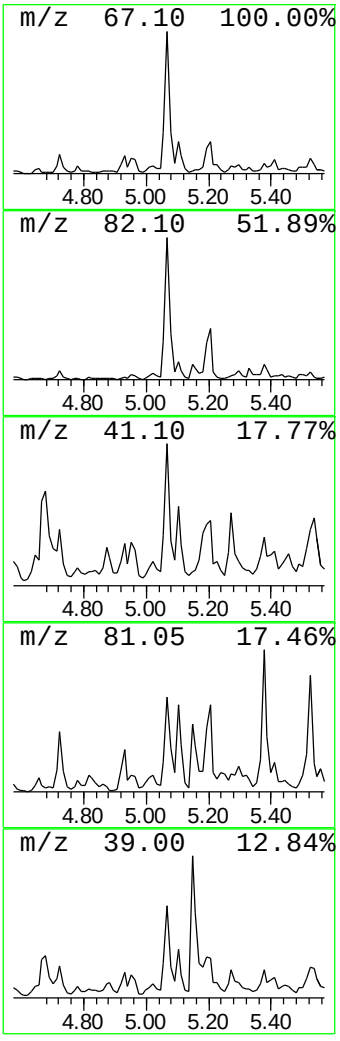
****

Peak Number 9 Pentalene, octahydro-, cis- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	9.68 ng	624695	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-, cis-	110	C8H14	001755-05-1	91
2	Pentalene, octahydro-	110	C8H14	000694-72-4	91
3	2,4-Hexadiene, (Z,Z)-	82	C6H10	006108-61-8	72
4	4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	72
5	4-Hexen-1-ol, acetate	142	C8H14O2	072237-36-6	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

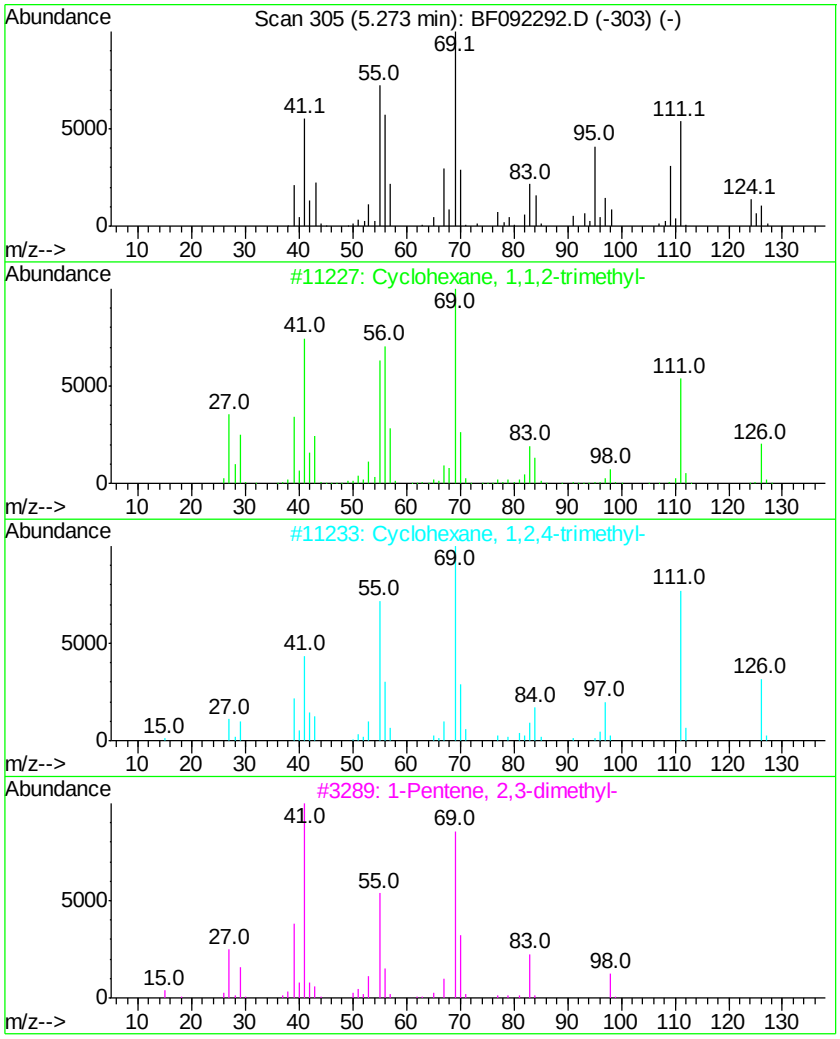
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

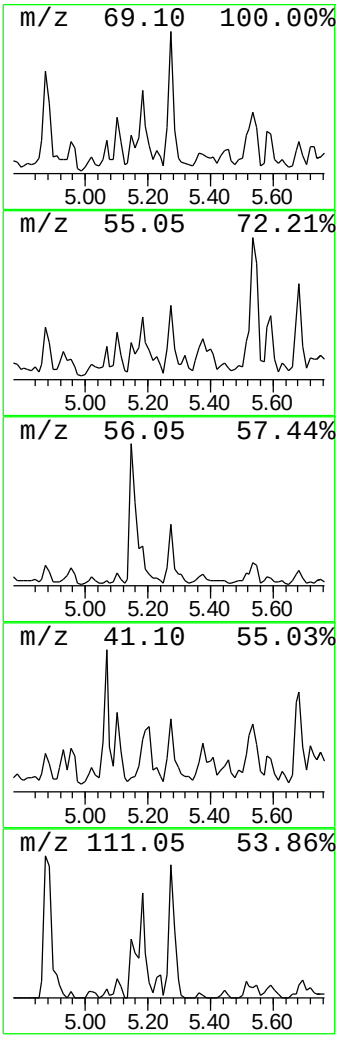
****

Peak Number 10 Cyclohexane, 1,1,2-trimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	4.90 ng	316354	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	70
2	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	60
3	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	27
4	2-Heptene, 2,6-dimethyl-	126	C9H18	005557-98-2	25
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

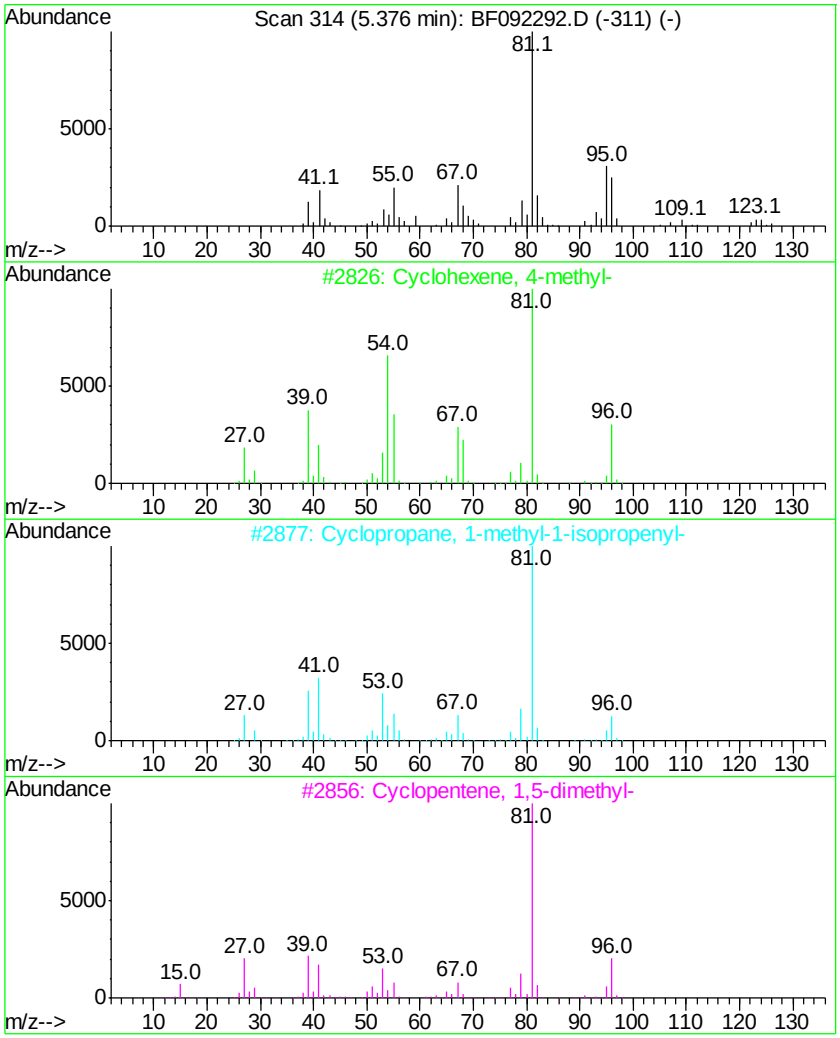
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

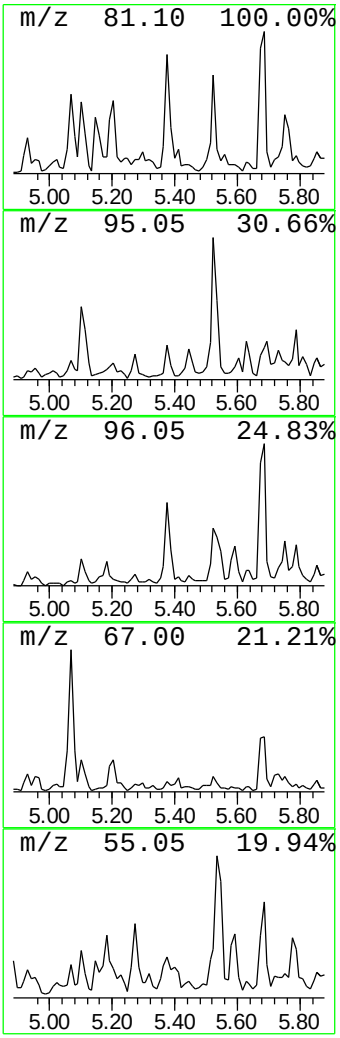
****

Peak Number 11 Cyclohexene, 4-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	5.09 ng	328465	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	64
2	Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	53
3	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	53
4	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	53
5	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

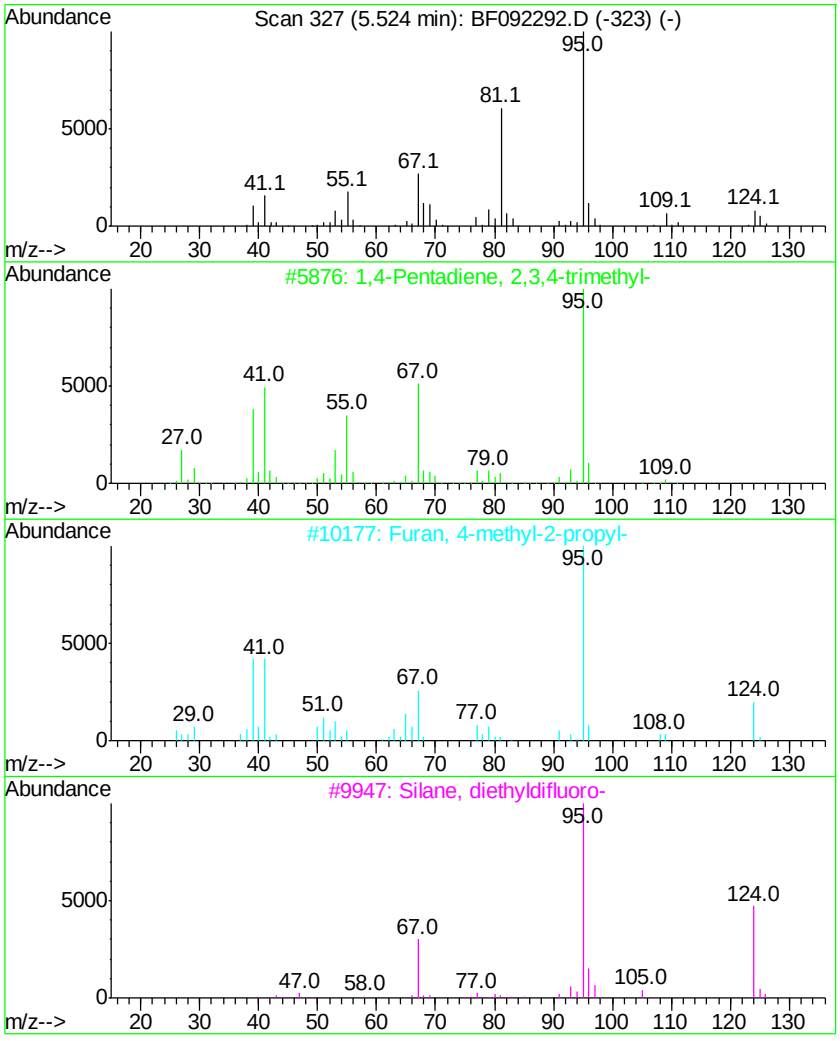
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

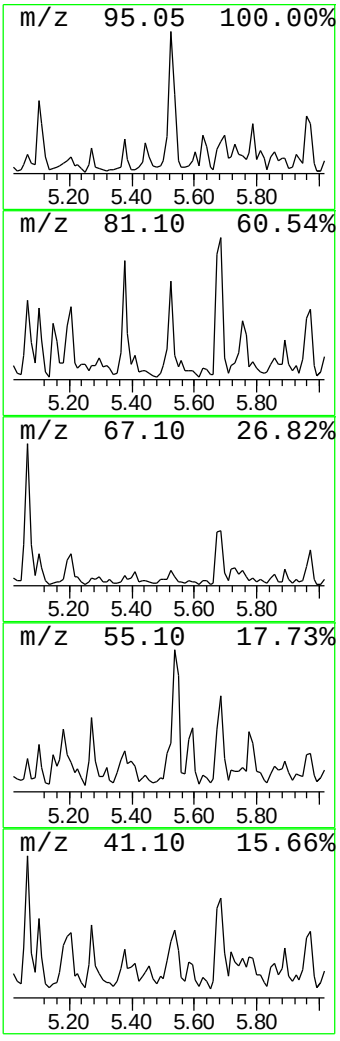
****

Peak Number 12 1,4-Pentadiene, 2,3,4-trime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	10.15 ng	654905	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	64
2	Furan, 4-methyl-2-propyl-	124	C8H12O	006148-37-4	64
3	Silane, diethyldifluoro-	124	C4H10F2Si	000358-06-5	59
4	exo-2-Bromonorbornane	174	C7H11Br	002534-77-2	53
5	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

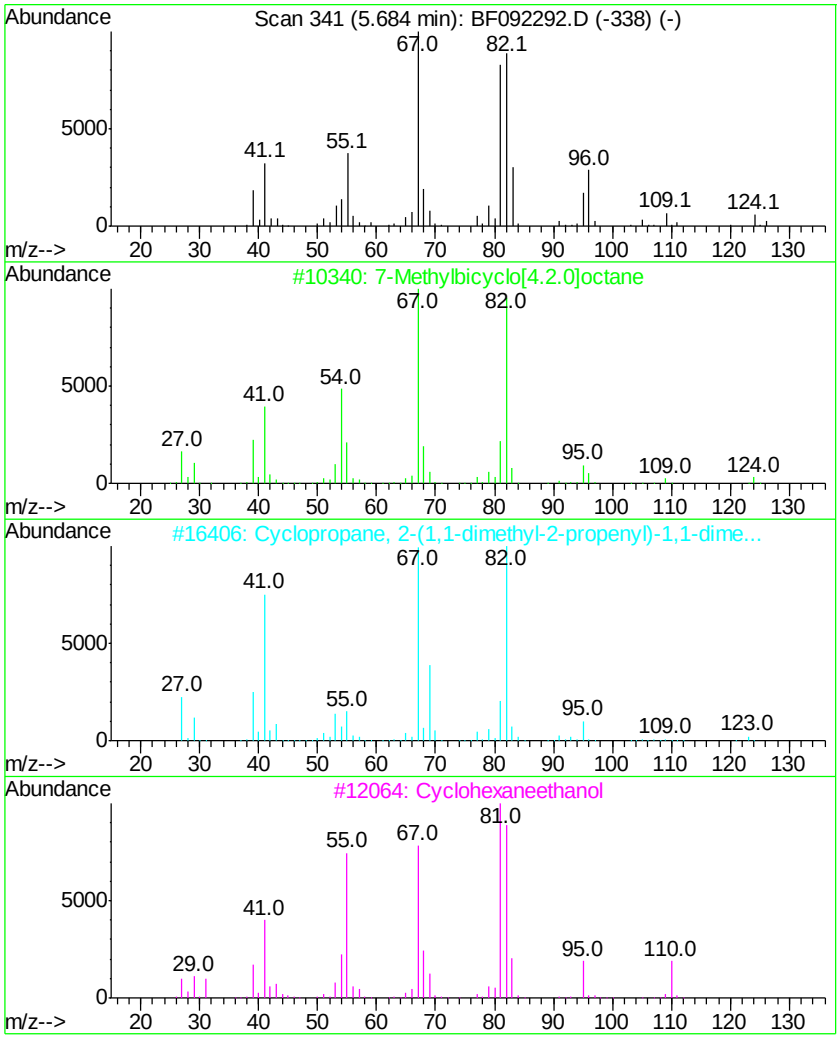
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

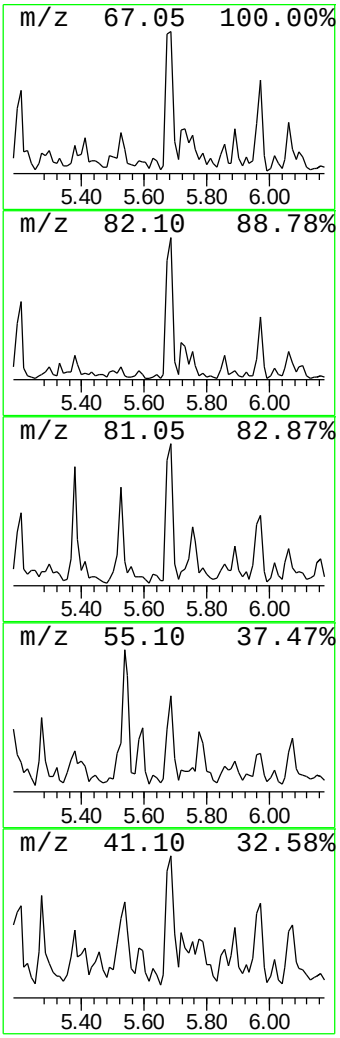
****

Peak Number 13 7-Methylbicyclo[4.2.0]octane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	20.19 ng	1302810	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methylbicyclo[4.2.0]octane	124	C9H16	1000210-90-2	58
2	Cyclopropane, 2-(1,1-dimethyl-2-...	138	C10H18	081051-15-2	47
3	Cyclohexaneethanol	128	C8H16O	004442-79-9	43
4	Cis-bicyclo[4.2.0]octane	110	C8H14	028282-35-1	43
5	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

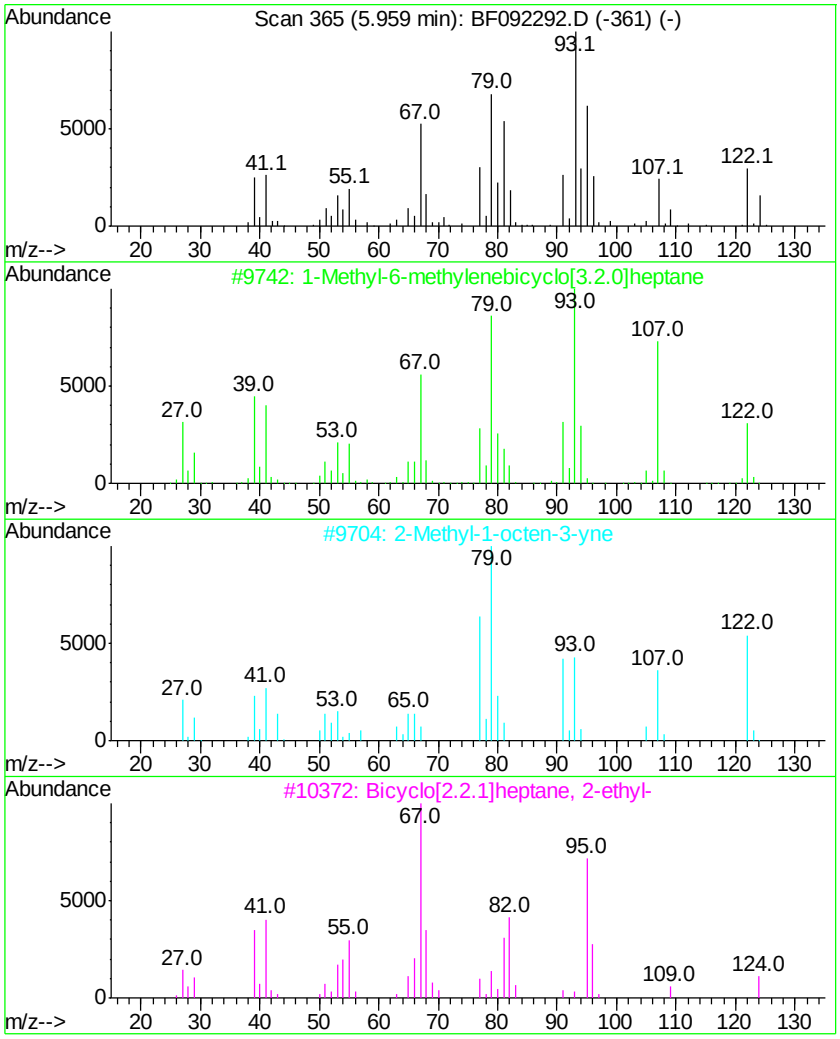
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

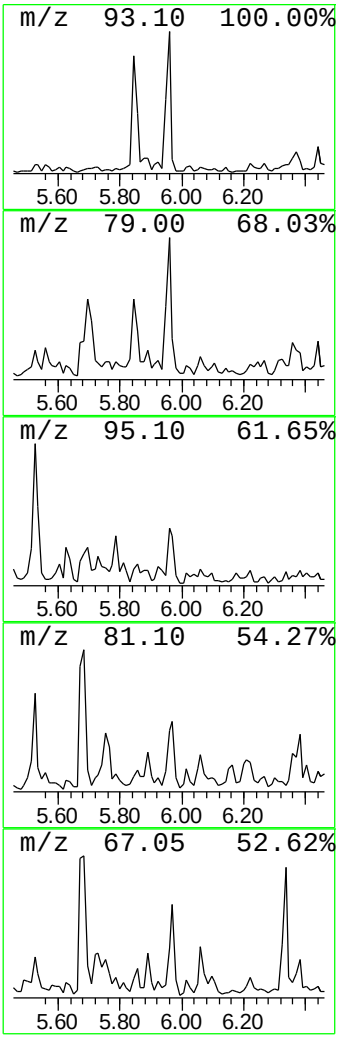
****

Peak Number 14 1-Methyl-6-methylenebicyclo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.96	10.65 ng	687031	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-6-methylenebicyclo[3.2....	122	C9H14	1000210-90-0	58
2	2-Methyl-1-octen-3-yne	122	C9H14	017603-76-8	25
3	Bicyclo[2.2.1]heptane, 2-ethyl-	124	C9H16	002146-41-0	22
4	4,4-Dimethylcyclohexadienone	122	C8H10O	001073-14-9	18
5	1,3,5-Heptatriene, (E,E)-	94	C7H10	017679-93-5	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

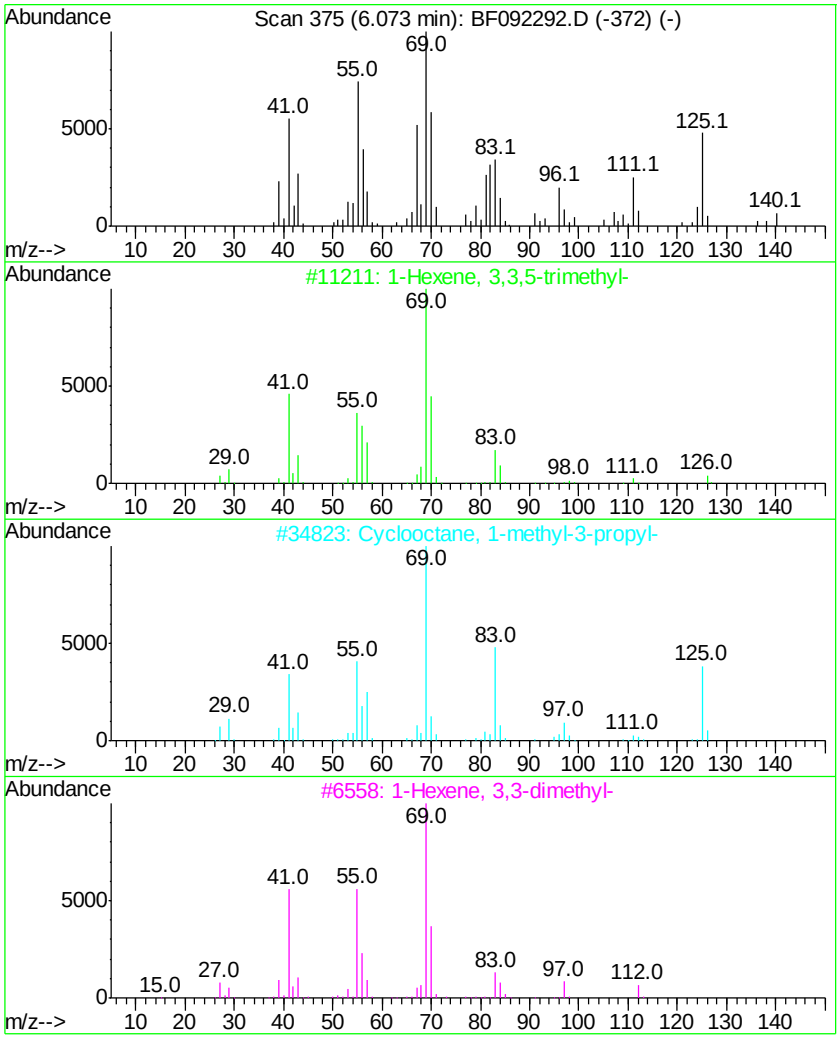
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

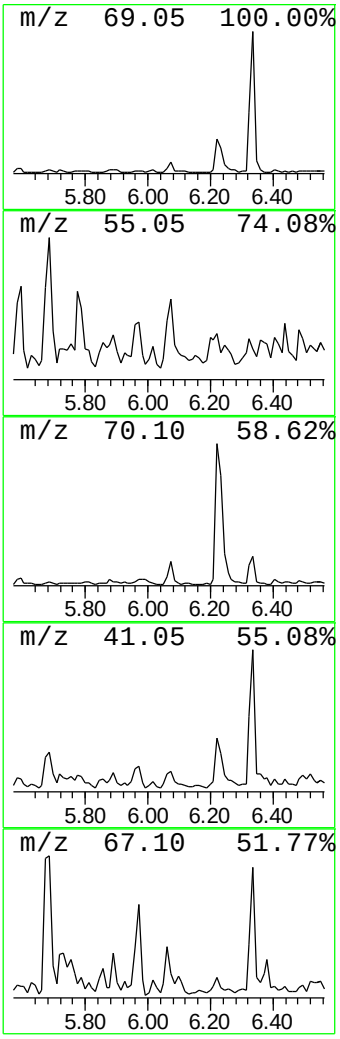
****

Peak Number 15 unknown6.07 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.07	5.37 ng	346880	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	46
2	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	43
3	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	38
4	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	35
5	3-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

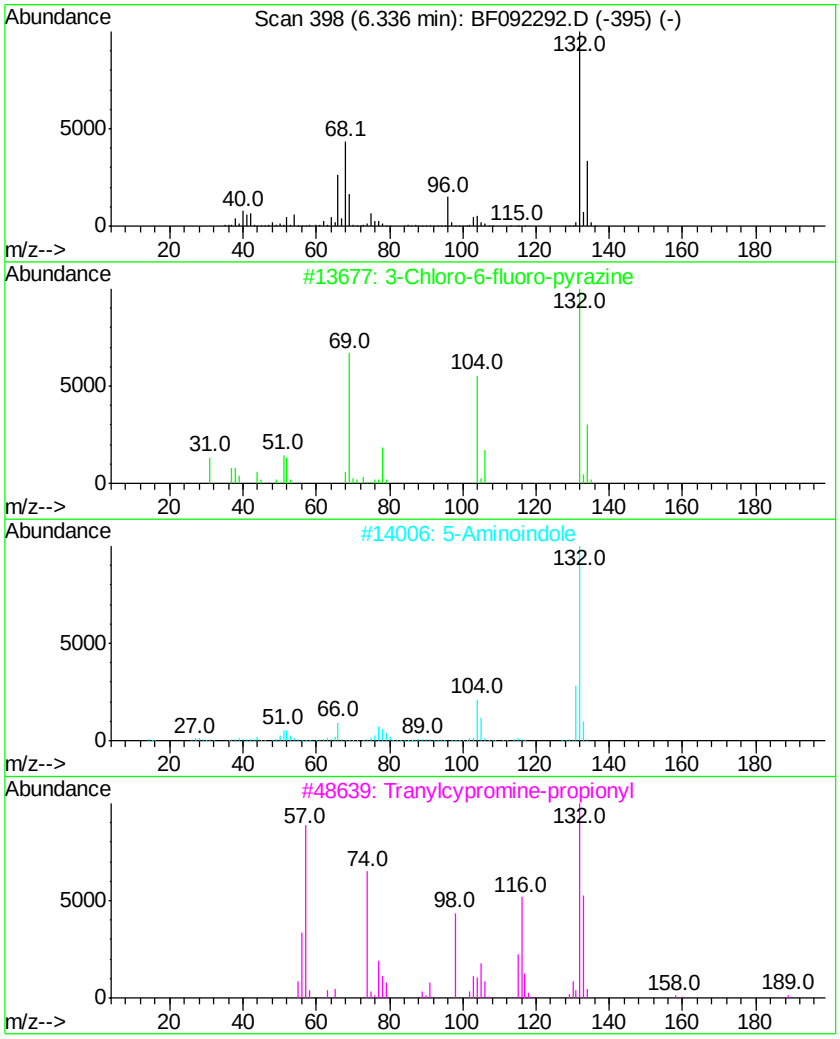
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

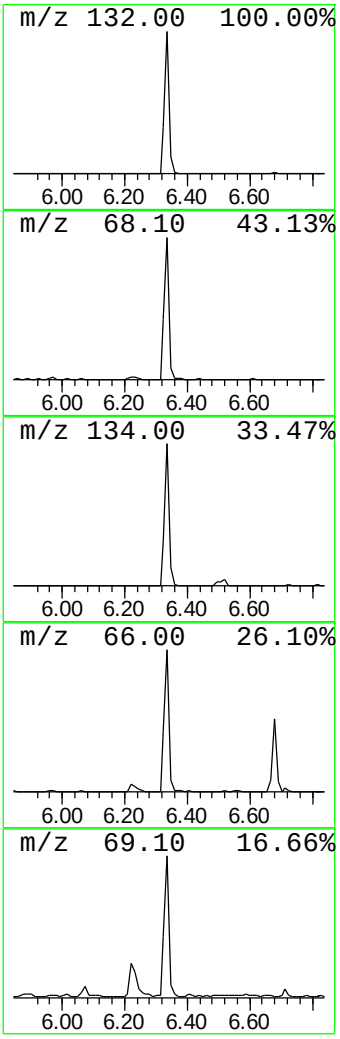
****

Peak Number 16 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	87.85 ng	5669870	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

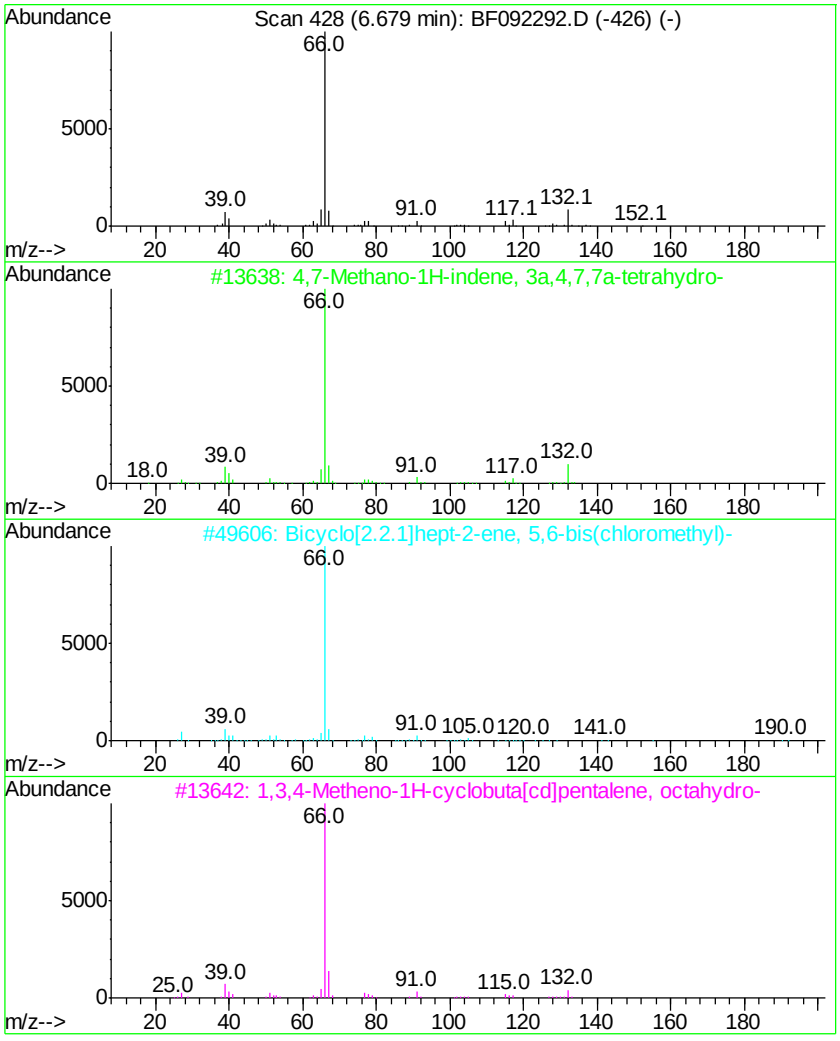
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

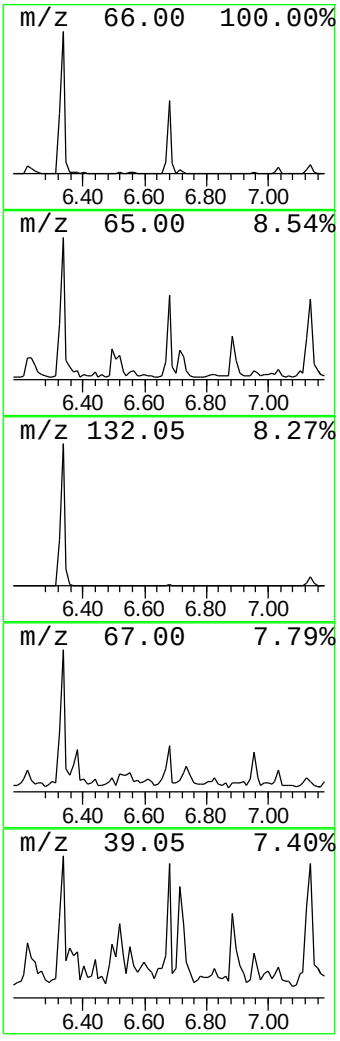
****

Peak Number 17 4,7-Methano-1H-indene, 3a,4... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	4.36 ng	281657	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-1H-indene, 3a,4,7,7a...	132	C10H12	000077-73-6	91
2	Bicyclo[2.2.1]hept-2-ene, 5,6-bi...	190	C9H12Cl2	005992-56-3	83
3	1,3,4-Metheno-1H-cyclobuta[cd]pe...	132	C10H12	006707-88-6	83
4	2-Norbornene	94	C7H10	000498-66-8	74
5	Bicyclo[2.2.1]hept-2-ene, 5-ethe...	120	C9H12	003048-64-4	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

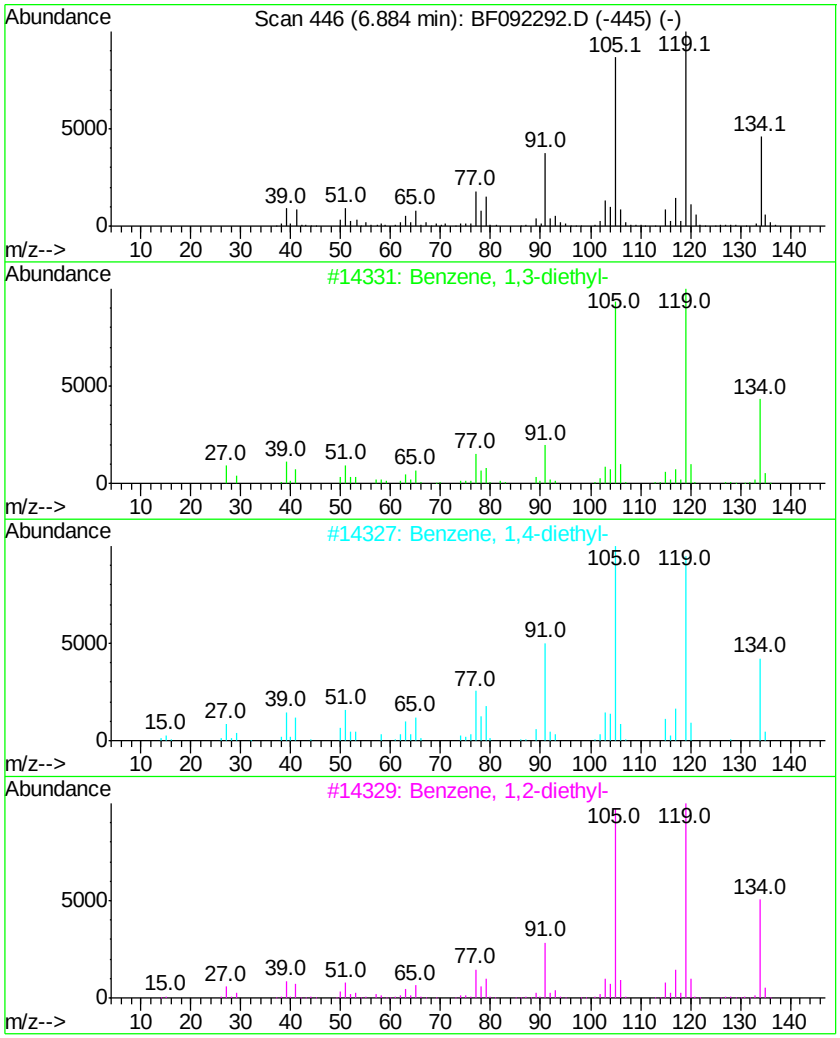
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

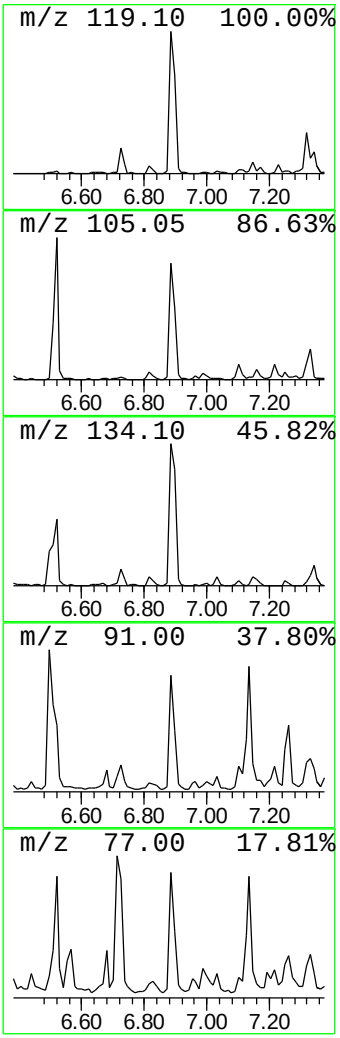
****

Peak Number 19 Benzene, 1,3-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	11.00 ng	709984	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	97
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	90
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

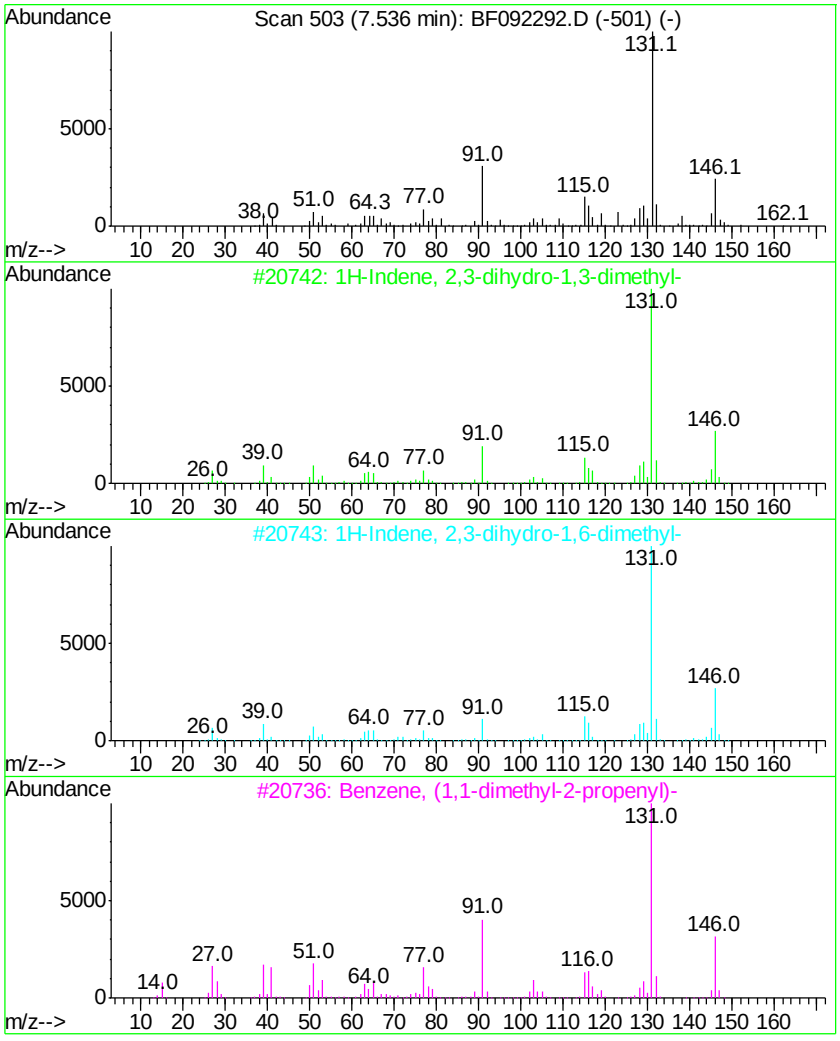
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

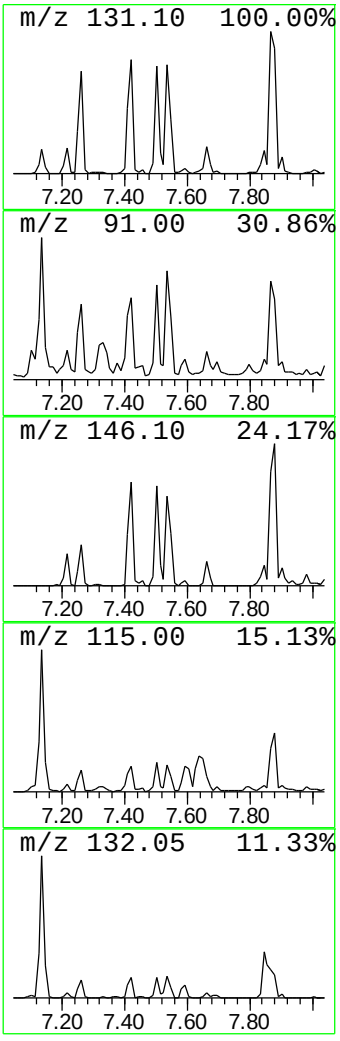
****

Peak Number 20 1H-Indene, 2,3-dihydro-1,3-... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	4.17 ng	538752	Naphthalene-d8	7.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	95
2	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94
3	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	93
4	1H-Indene,2,3-dihydro-2,2-dimethyl-	146	C11H14	020836-11-7	91
5	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092292.D
Acq On : 16 Jan 2017 18:35
Operator : UM/SJ
Sample : I1196-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-52

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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
Cyclopentane, 1,2...	2.60	4.3	ng	276560	1	6.56	1290770	20.0
1,4-Pentadiene, 2...	3.54	5.7	ng	365365	1	6.56	1290770	20.0
Cyclohexane, 1,1-...	3.72	7.4	ng	475655	1	6.56	1290770	20.0
Cyclohexane, 1,2-...	3.97	17.6	ng	1135950	1	6.56	1290770	20.0
1,3-Dimethyl-1-cy...	4.12	30.1	ng	1944470	1	6.56	1290770	20.0
Cyclohexene, 1,2-...	4.44	6.2	ng	401393	1	6.56	1290770	20.0
2-Pentanone, 4-hy...	4.68	21.0	ng	1353420	1	6.56	1290770	20.0
Pentalene, octahy...	5.07	9.7	ng	624695	1	6.56	1290770	20.0
Cyclohexane, 1,1,...	5.27	4.9	ng	316354	1	6.56	1290770	20.0
Cyclohexene, 4-me...	5.38	5.1	ng	328465	1	6.56	1290770	20.0
1,4-Pentadiene, 2...	5.52	10.2	ng	654905	1	6.56	1290770	20.0
7-Methylbicyclo[4...	5.68	20.2	ng	1302810	1	6.56	1290770	20.0
1-Methyl-6-methyl...	5.96	10.7	ng	687031	1	6.56	1290770	20.0
unknown6.07	6.07	5.4	ng	346880	1	6.56	1290770	20.0
unknown6.34	6.34	87.8	ng	5669870	1	6.56	1290770	20.0
4,7-Methano-1H-in...	6.68	4.4	ng	281657	1	6.56	1290770	20.0
Benzene, 1,3-diet...	6.88	11.0	ng	709984	1	6.56	1290770	20.0
1H-Indene, 2,3-di...	7.54	4.2	ng	538752	2	7.84	2585620	20.0