LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

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_M\METHODS\8270-BM051117.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	3.487	65	68	69	rVV	64175	73044	1.68%	0.132%
2	3.510	69	72	80	rVV	282168	357071	8.21%	0.645%
3	3.746	109	112	113	rVV	65622	82527	1.90%	0.149%
4	3.763	113	115	119	rVV	113715	151097	3.48%	0.273%
5	3.810	119	123	128	rVB	99466	134064	3.08%	0.242%
6	3.998	151	155	160	rVB2	55495	76060	1.75%	0.137%
7	4.263	196	200	202	rVV2	165044	229707	5.28%	0.415%
8	4.293	202	205	212	rVB	473688	635184	14.61%	1.148%
9	4.587	249	255	259	rBV2	46116	79671	1.83%	0.144%
10	4.687	267	272	279	rBV3	50273	95022	2.19%	0.172%
11	4.745	279	282	285	rBV2	48412	72428	1.67%	0.131%
12	4.898	304	308	310	rBV	87285	121401	2.79%	0.219%
13	4.922	310	312	316	rVV	83247	114681	2.64%	0.207%
14	4.981	316	322	328	rVB	340226	558929	12.86%	1.010%
15	5.251	363	368	377	rVB5	55488	129853	2.99%	0.235%
16	5.351	377	385	397	rBV	767253	1238217	28.48%	2.238%
17	5.663	432	438	443	rBV2	467622	742026	17.07%	1.341%
18	5.757	449	454	458	rBV3	68906	120774	2.78%	0.218%
19	5.810	458	463	467	rVV	166910	234651	5.40%	0.424%
20	6.045	498	503	512	rVB	1214062	1766115	40.62%	3.191%
21	6.240	531	536	548	rVB2	125888	272519	6.27%	0.492%
22	6.516	573	583	592	rBV2	1414777	2339041	53.80%	4.227%
23	6.622	592	601	605	rBV5	35244	82535	1.90%	0.149%
24	6.663	605	608	614	rVB5	42395	76556	1.76%	0.138%
25	6.728	614	619	623	rBV	221034	330728	7.61%	0.598%
26	6.828	631	636	650	rVB3	315530	659193	15.16%	1.191%
27	6.951	650	657	664	rBV	430463	826881	19.02%	1.494%
28	7.022	664	669	673	rBV	305919	457213	10.52%	0.826%
29	7.169	685	694	697	rBV4	63268	136864	3.15%	0.247%
30	7.216	697	702	709	rVB4	56940	94174	2.17%	0.170%
31	7.298	709	716	721	rBV	1257321	2065243	47.50%	3.732%
32	7.628	756	772	782	rBV6	275964	1002188	23.05%	1.811%
33	7.722	782	788	789	rBV3	69791	99943	2.30%	0.181%
34	7.757	789	794	799	rVB2	271006	451643	10.39%	0.816%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

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_M\METHODS\8270-BM051117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.822	799	805	818	rVB	1394930	2357651	54.23%	4.260%
36	7.986	818	833	836	rBV5	134121	485490	11.17%	0.877%
37	8.075	838	848	852	rBV	1260873	2419804	55.66%	4.373%
38	8.122	852	856	860	rVB	934613	1265954	29.12%	2.288%
39	8.175	861	865	867	rBV3	143895	239699	5.51%	0.433%
40	8.234	871	875	879	rBV2	413788	779864	17.94%	1.409%
41	8.381	895	900	904	rVV	185244	319988	7.36%	0.578%
42	8.428	904	908	915	rVB5	152733	279151	6.42%	0.504%
43	8.545	924	928	930	rBV	49461	79455	1.83%	0.144%
44	8.692	947	953	958	rBV4	133156	219328	5.04%	0.396%
45	8.739	958	961	966	rVB3	82388	115412	2.65%	0.209%
46	8.845	966	979	983	rBV	1039529	2218478	51.03%	4.009%
47	8.933	988	994	999	rVB3	1456685	2677833	61.59%	4.839%
48	9.010	1001	1007	1010	rBV5	489539	950749	21.87%	1.718%
49	9.157	1030	1032	1035	rVB2	87107	71706	1.65%	0.130%
50	9.269	1045	1051	1058	rBV6	107002	252750	5.81%	0.457%
51	9.369	1063	1068	1075	rVV	338539	559809	12.88%	1.012%
52	9.557	1082	1100	1107	rBV8	406790	1426983	32.82%	2.579%
53	9.622	1107	1111	1116	rVB3	66517	94252	2.17%	0.170%
54	9.733	1125	1130	1134	rBV6	81139	153485	3.53%	0.277%
55	9.792	1134	1140	1147	rVB2	321953	583459	13.42%	1.054%
56	9.939	1154	1165	1185	rBV2	666335	1512534	34.79%	2.733%
57	10.116	1185	1195	1198	rBV10	72084	188199	4.33%	0.340%
58	10.163	1198	1203	1211	rVV3	124211	299963	6.90%	0.542%
59	10.239	1211	1216	1221	rVV	50494	76284	1.75%	0.138%
60	10.516	1260	1263	1265	rVV3	108091	151166	3.48%	0.273%
61	10.551	1265	1269	1282	rVV2	337664	811438	18.66%	1.466%
62	10.651	1282	1286	1292	rVB3	94235	159256	3.66%	0.288%
63	10.751	1300	1303	1308	rVB4	68709	107301	2.47%	0.194%
64	10.857	1308	1321	1325	rBV10	59815	198430	4.56%	0.359%
65	10.980	1337	1342	1352	rVB10	77069	203368	4.68%	0.368%
66	11.198	1374	1379	1383	rVV3	72930	146081	3.36%	0.264%
67	11.245	1385	1387	1392	rVB4	52393	80167	1.84%	0.145%
68	11.457	1412	1423	1429	rBV2	83320	174940	4.02%	0.316%
69	11.551	1433	1439	1443	rBV6	36309	78972	1.82%	0.143%
70	11.645	1452	1455	1461	rVB3	63804	105345	2.42%	0.190%
71	12.116	1529	1535	1540	rVB7	45643	90163	2.07%	0.163%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

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_M\METHODS\8270-BM051117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.298	1561	1566	1570	rVB2	109848	175073	4.03%	0.316%
73	12.451	1577	1592	1598	rBV4	254225	567661	13.06%	1.026%
74	12.604	1612	1618	1624	rVB	98577	160305	3.69%	0.290%
75	12.721	1633	1638	1640	rBV5	54590	84178	1.94%	0.152%
76	12.751	1641	1643	1651	rVB3	72679	114880	2.64%	0.208%
77	12.874	1659	1664	1670	rVV3	72268	137094	3.15%	0.248%
78	13.021	1682	1689	1696	rBV	2422701	3482821	80.11%	6.294%
79	13.116	1701	1705	1713	rVB9	32278	71591	1.65%	0.129%
80	13.227	1721	1724	1729	rVB3	53833	82548	1.90%	0.149%
81	13.392	1745	1752	1757	rBV7	53427	98967	2.28%	0.179%
82	13.463	1757	1764	1772	rVV6	62899	120343	2.77%	0.217%
83	13.557	1774	1780	1785	rBV6	111446	196676	4.52%	0.355%
84	13.627	1785	1792	1799	rVB2	134818	264277	6.08%	0.478%
85	13.727	1801	1809	1813	rBV2	95853	173583	3.99%	0.314%
86	13.780	1815	1818	1825	rVB7	68125	118198	2.72%	0.214%
87	13.921	1837	1842	1846	rBV3	118718	207911	4.78%	0.376%
88	14.057	1859	1865	1871	rVB8	41763	76918	1.77%	0.139%
89	14.245	1890	1897	1903	rBV7	39167	78483	1.81%	0.142%
90	14.415	1917	1926	1936	rVB2	520692	887437	20.41%	1.604%
91	15.068	2033	2037	2043	rVB7	50950	99930	2.30%	0.181%
92	15.168	2043	2054	2061	rBV10	48452	118791	2.73%	0.215%
93	15.915	2175	2181	2189	rBV	1957829	2782646	64.00%	5.028%
94	17.168	2388	2394	2401	rBV	688571	959384	22.07%	1.734%
95	18.045	2537	2543	2550	rBV2	105942	173926	4.00%	0.314%
96	19.327	2757	2761	2765	rBV3	53617	70975	1.63%	0.128%
97	19.792	2834	2840	2846	rBV	3665263	4347803	100.00%	7.857%
98	21.044	3049	3053	3058	rBV7	69867	101624	2.34%	0.184%
99	21.356	3101	3106	3114	rVB	767344	975257	22.43%	1.762%
100	23.650	3490	3496	3504	rVB	407910	766675	17.63%	1.385%

Sum of corrected areas: 55338105

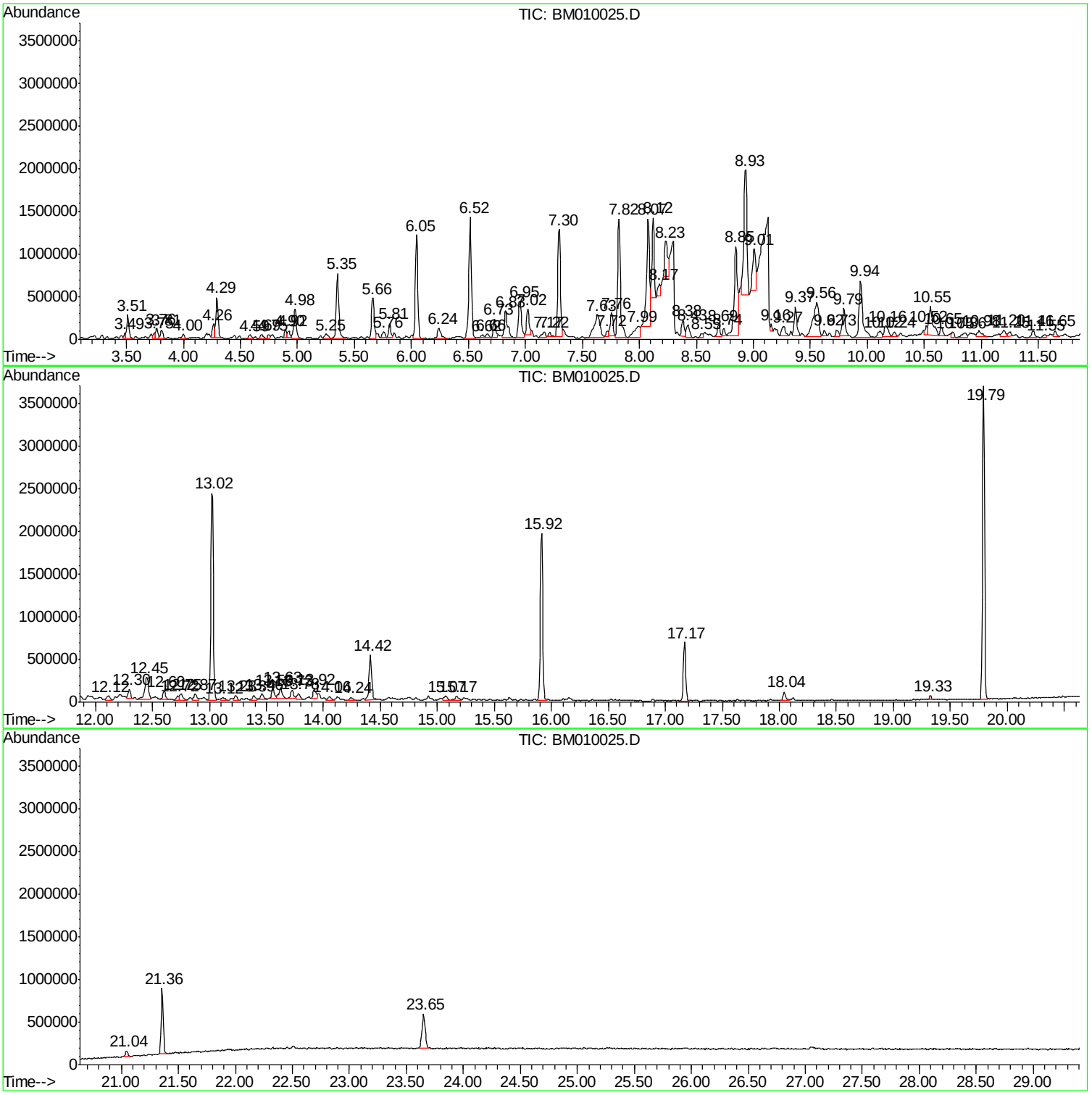
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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 M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

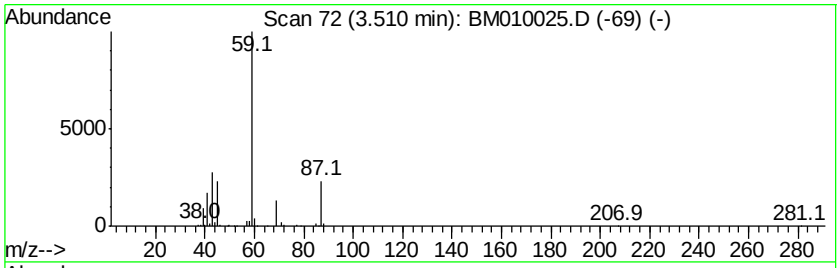
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

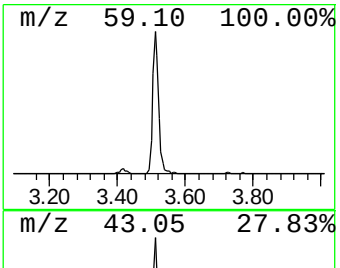
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.51	15.81 ng	357071	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	64
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
5	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	40





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

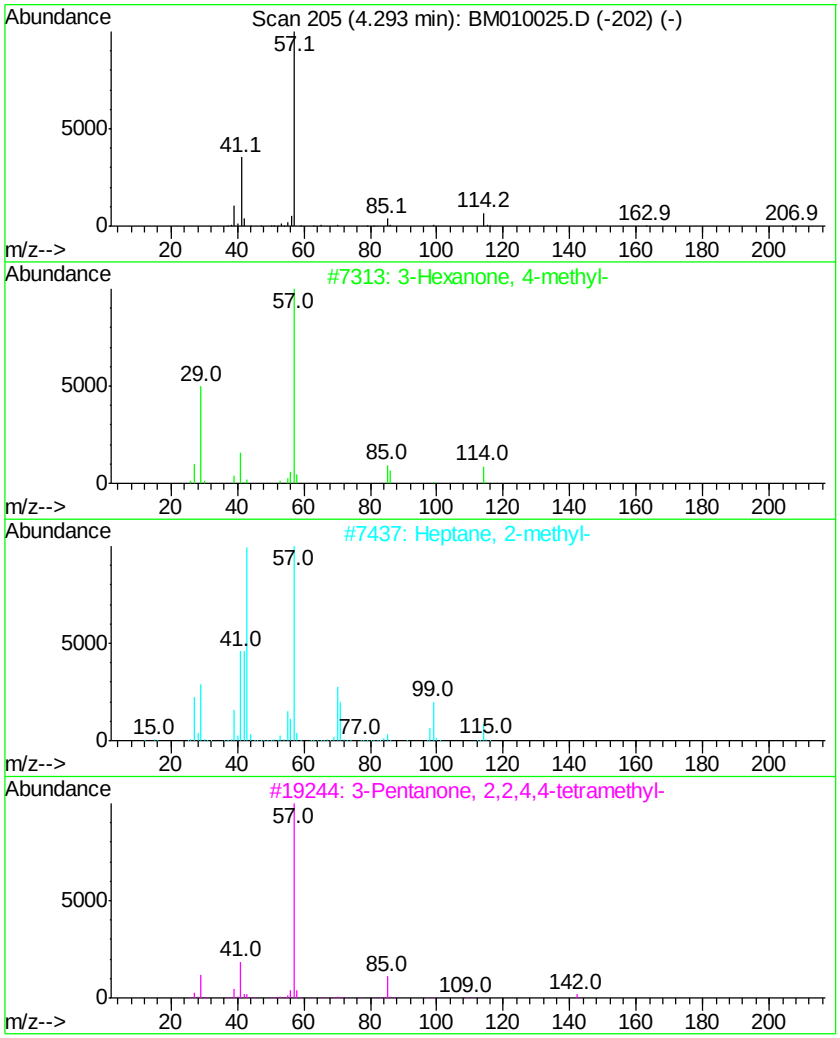
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

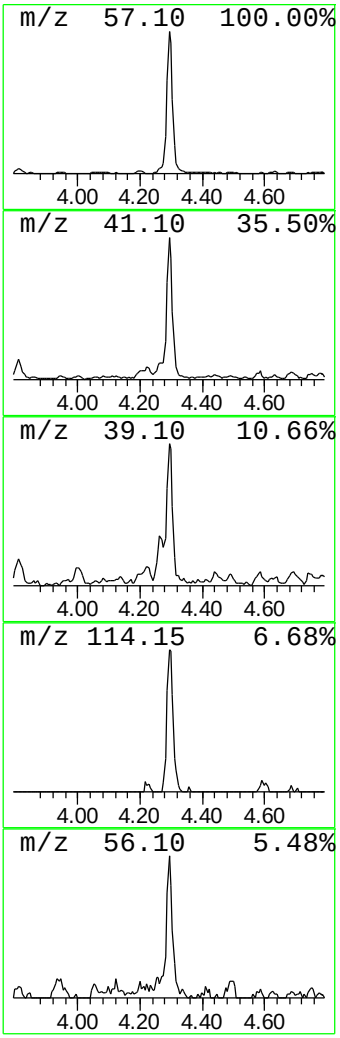
****

Peak Number 2 unknown4.29 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	28.13 ng	635184	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	9
2	Heptane, 2-methyl-	114	C8H18	000592-27-8	9
3	3-Pentanone, 2,2,4,4-tetramethyl-	142	C9H18O	000815-24-7	9
4	Pivalic acid vinyl ester	128	C7H12O2	003377-92-2	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

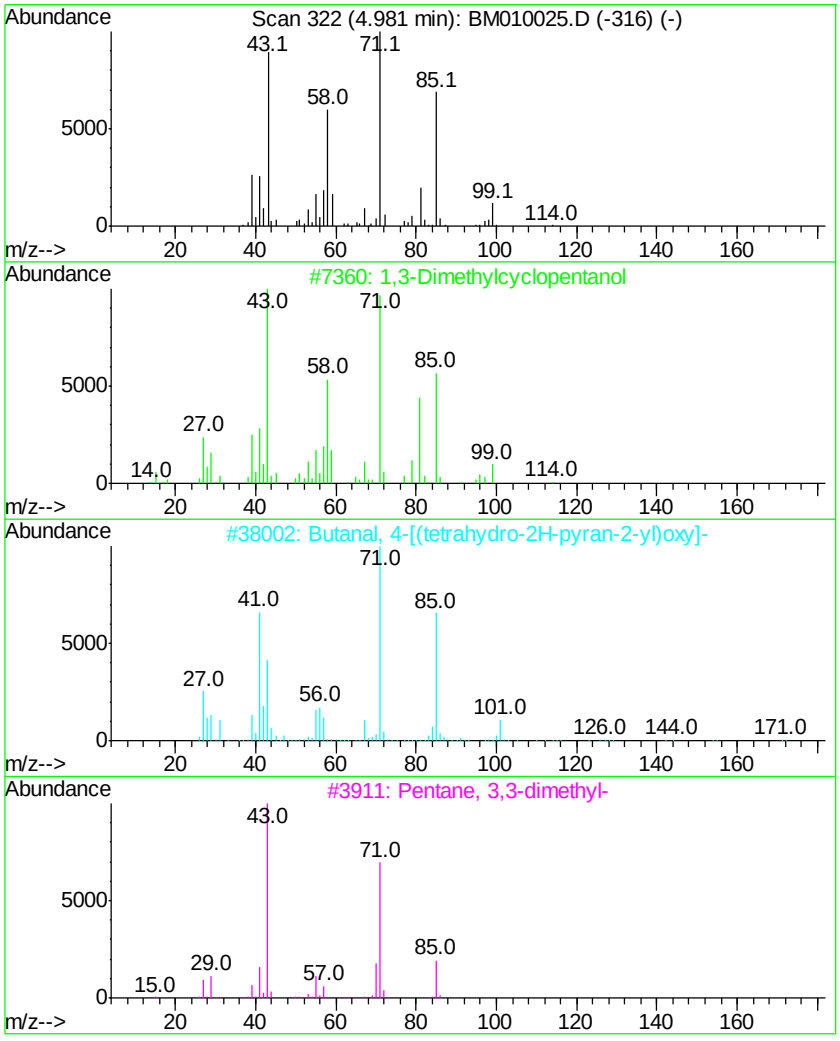
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

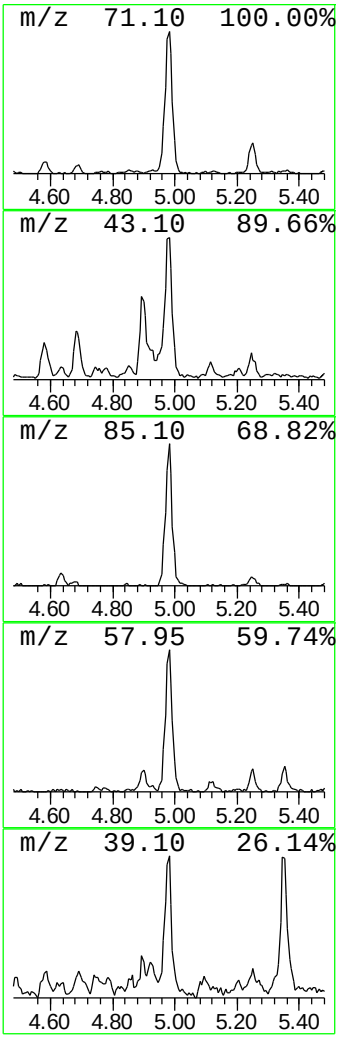
****

Peak Number 3 1,3-Dimethylcyclopentanol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	24.75 ng	558929	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	91
2	Butanal, 4-[(tetrahydro-2H-pyran...	172	C9H16O3	054911-85-2	50
3	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	50
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	43
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	38





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

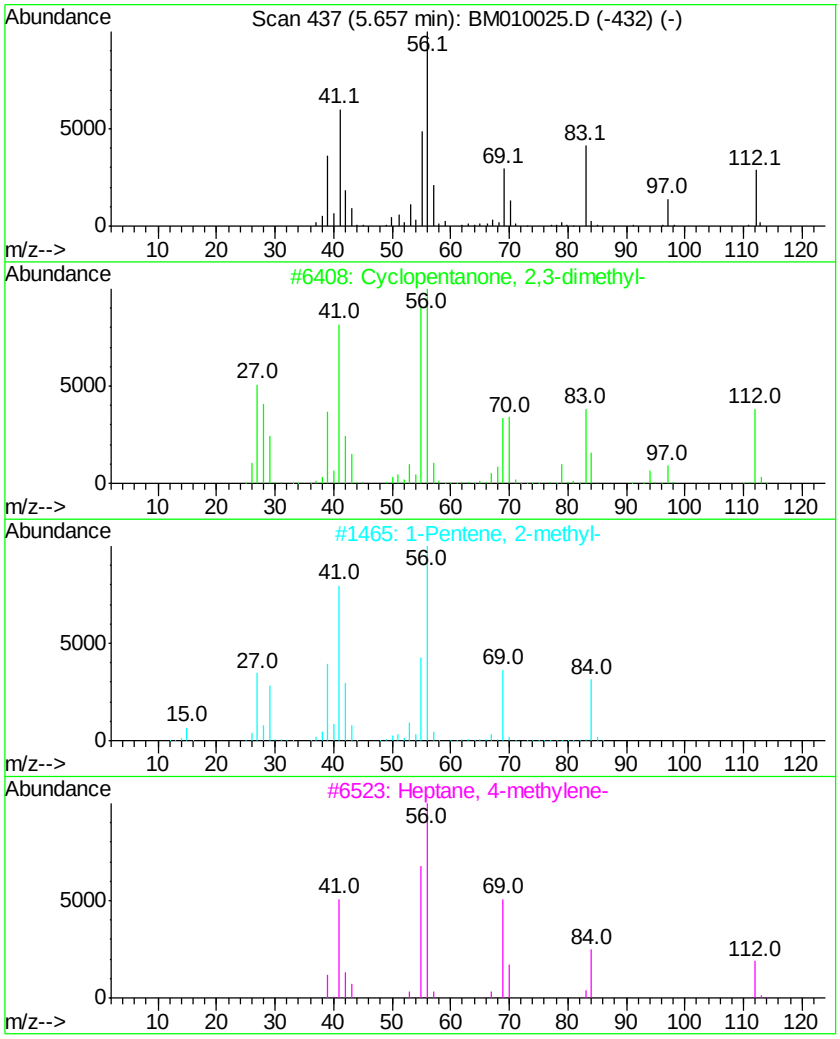
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

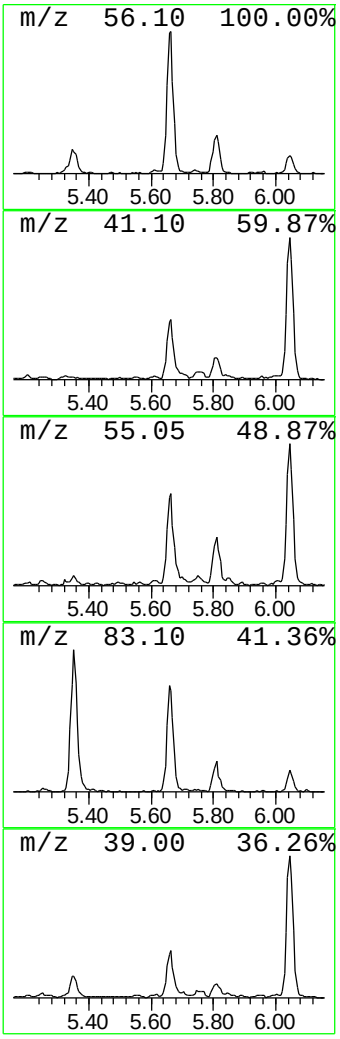
****

Peak Number 4 Cyclopentanone, 2,3-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.66	32.86 ng	742026	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone, 2,3-dimethyl-	112	C7H12O	1000151-06-7	50
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	49
3	Heptane, 4-methylene-	112	C8H16	015918-08-8	49
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47
5	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	43





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

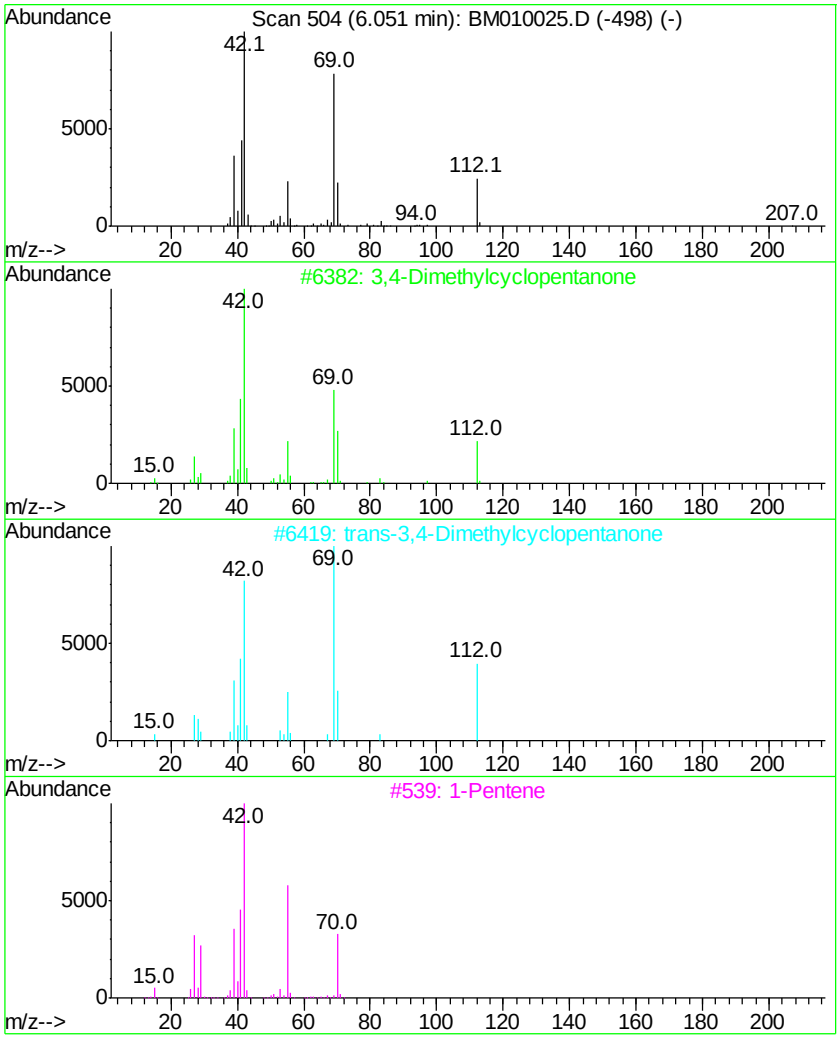
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

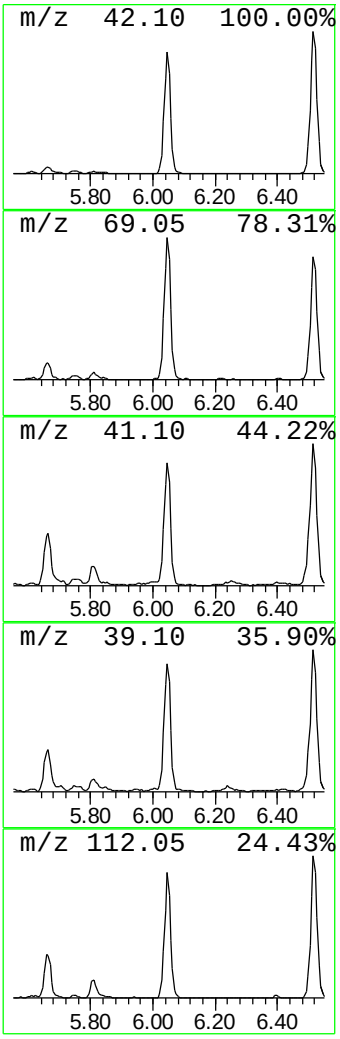
****

Peak Number 5 3,4-Dimethylcyclopentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.05	78.21 ng	1766120	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylcyclopentanone	112	C7H12O	058372-16-0	70
2	trans-3,4-Dimethylcyclopentanone	112	C7H12O	019550-73-3	64
3	1-Pentene	70	C5H10	000109-67-1	43
4	1,3-Cyclohexanedione	112	C6H8O2	000504-02-9	38
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	38





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Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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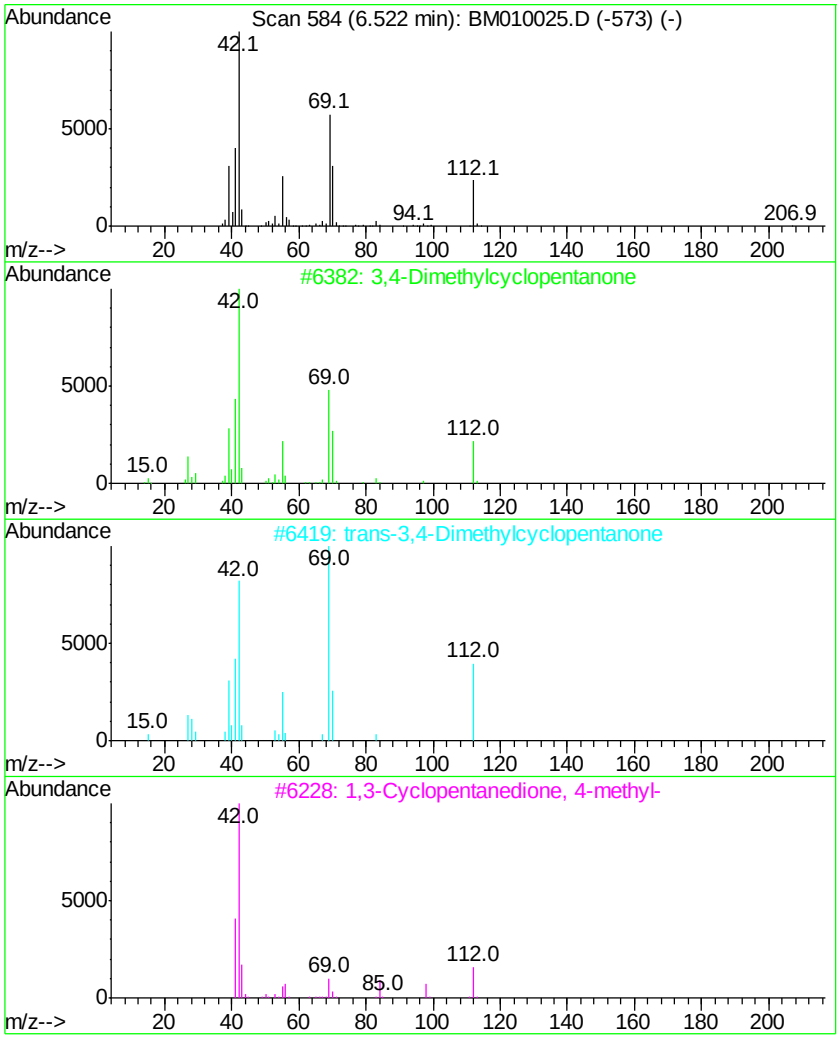
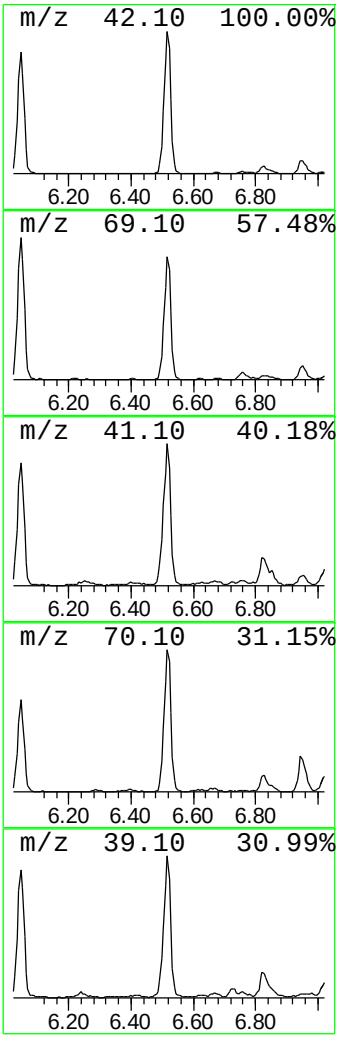
Peak Number 6 trans-3,4-Dimethylcyclopent... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	103.58 ng	2339040	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylcyclopentanone	112	C7H12O	058372-16-0	94
2	trans-3,4-Dimethylcyclopentanone	112	C7H12O	019550-73-3	72
3	1,3-Cyclopentanedione, 4-methyl-	112	C6H8O2	035029-03-9	64
4	1,3-Cyclohexanedione	112	C6H8O2	000504-02-9	64
5	4-Morpholinecarbonitrile	112	C5H8N2O	001530-89-8	59





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Sample : I3098-01
Misc :
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Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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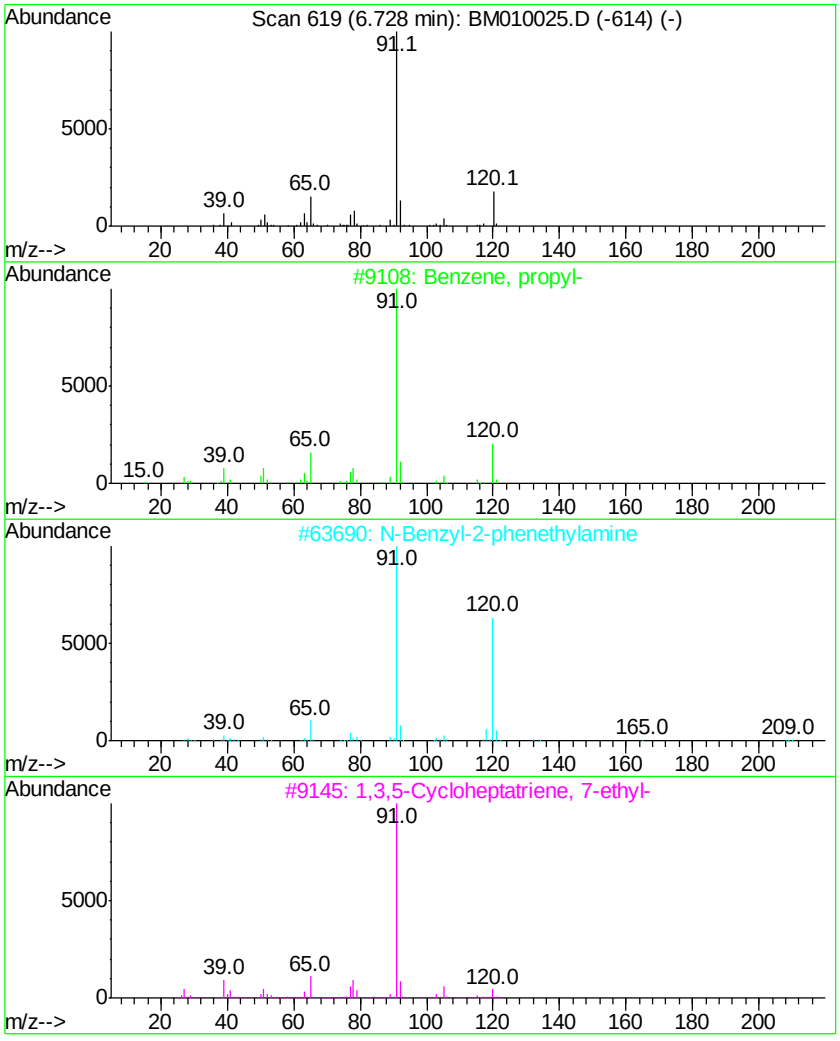
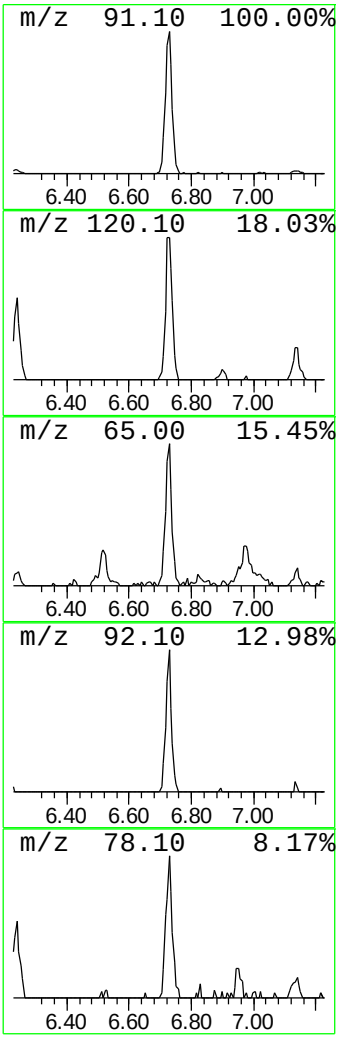
Peak Number 7 Benzene, propyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	14.65 ng	330728	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	95
2	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	78
3	1,3,5-Cycloheptatriene, 7-ethyl-	120	C9H12	017634-51-4	64
4	Benzene, (ethenyloxy)-	120	C8H8O	000766-94-9	59
5	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	53





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Instrument : BNA_M
ClientSampleId : MW-1R

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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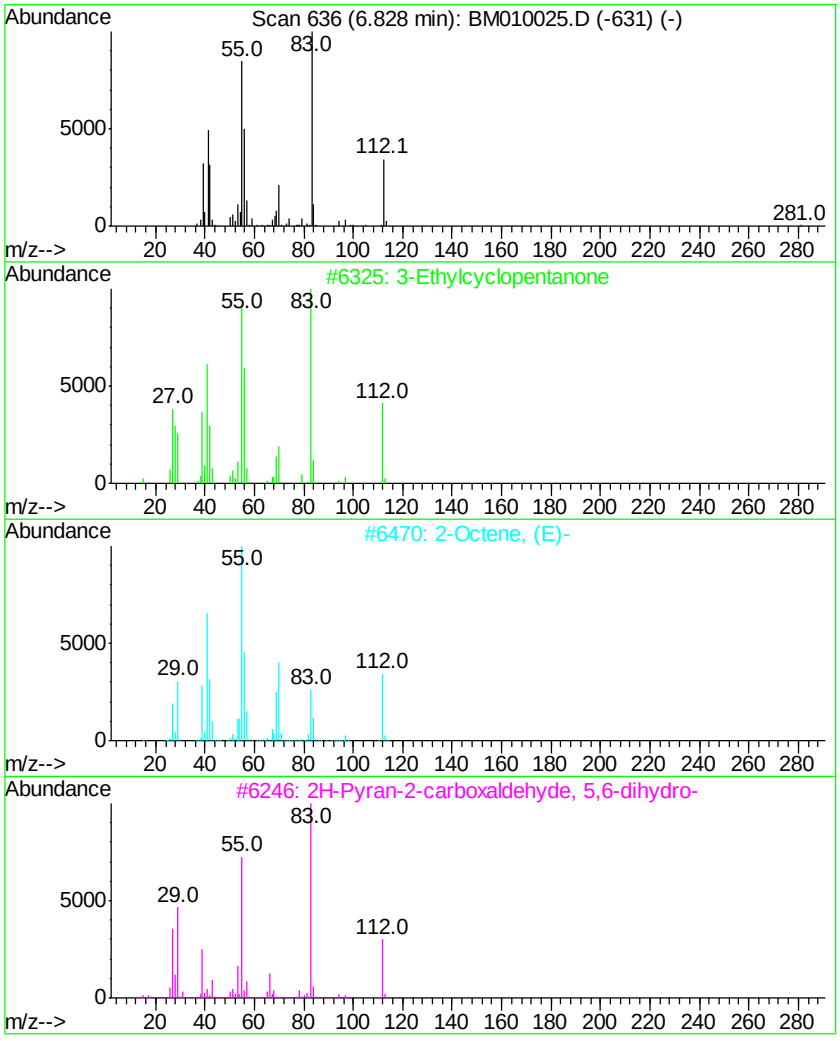
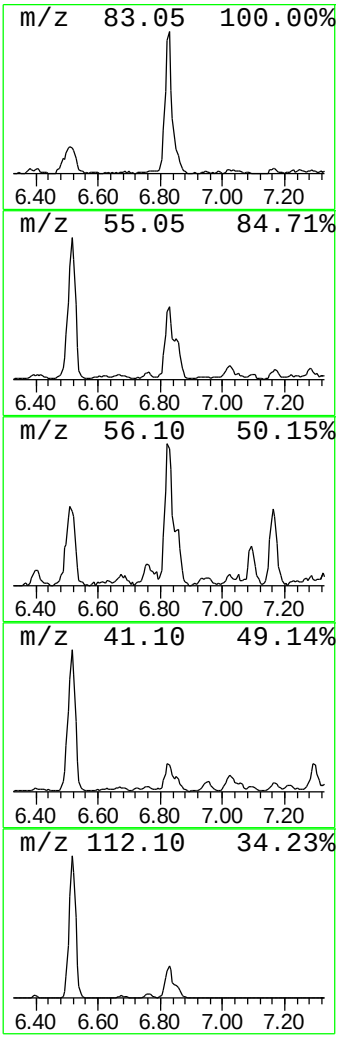
Peak Number 8 3-Ethylcyclopentanone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	29.19 ng	659193	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylcyclopentanone	112	C7H12O	010264-55-8	90
2	2-Octene, (E)-	112	C8H16	013389-42-9	53
3	2H-Pyran-2-carboxaldehyde, 5,6-d...	112	C6H8O2	053897-26-0	52
4	2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	52
5	Cyclohexane, ethyl-	112	C8H16	001678-91-7	52





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Misc :
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Instrument : BNA_M
ClientSampleId : MW-1R

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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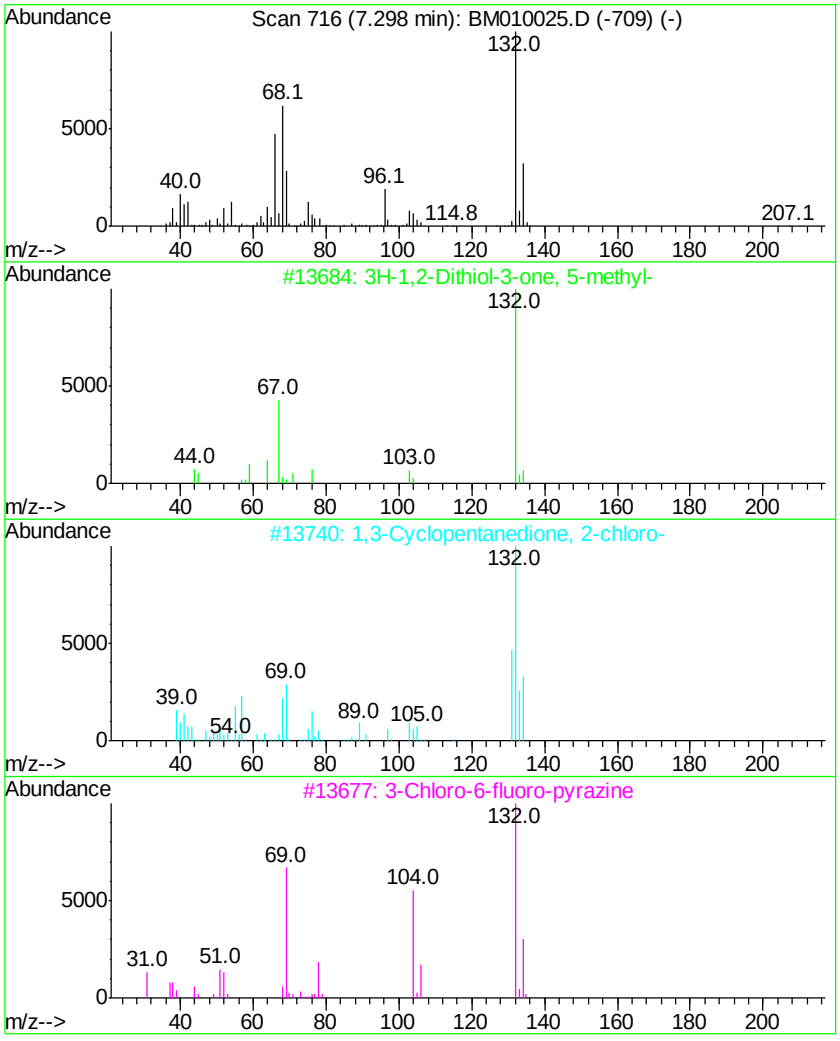
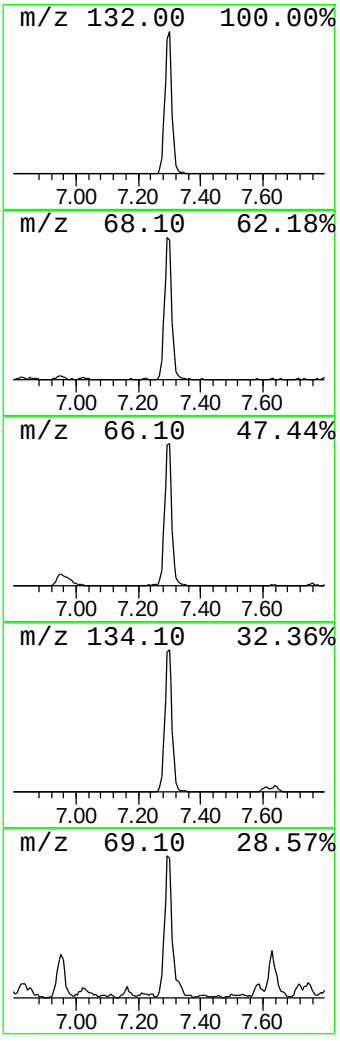
Peak Number 9 3H-1,2-Dithiol-3-one, 5-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	91.45 ng	2065240	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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ClientSampleId : MW-1R

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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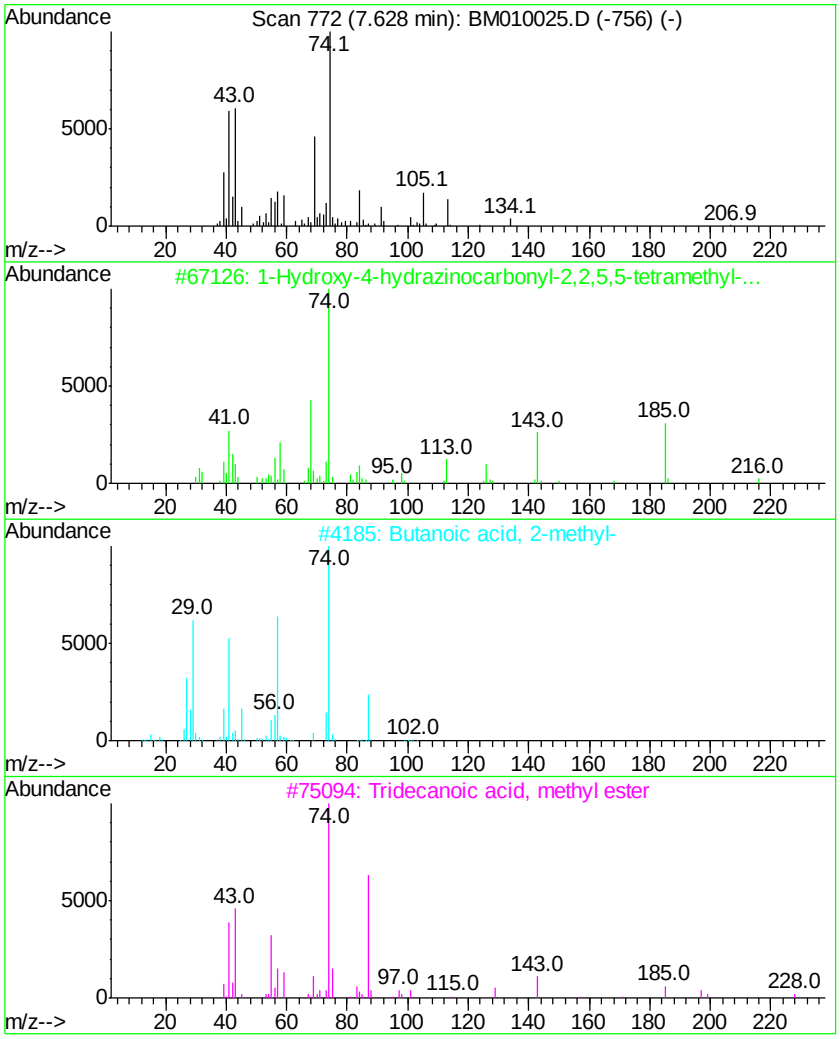
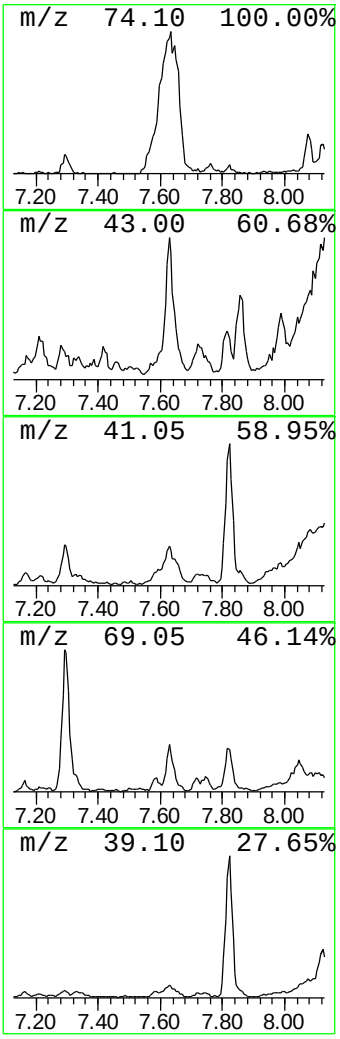
Peak Number 10 1-Hydroxy-4-hydrazinocarbon... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	44.38 ng	1002190	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hydroxy-4-hydrazinocarbonyl-2,...	216	C8H16N4O3	095057-50-4	59
2	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	38
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	36
4	Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	36
5	.beta.-d-Allopyranoside, methyl ...	192	C8H16O5	014917-72-7	33





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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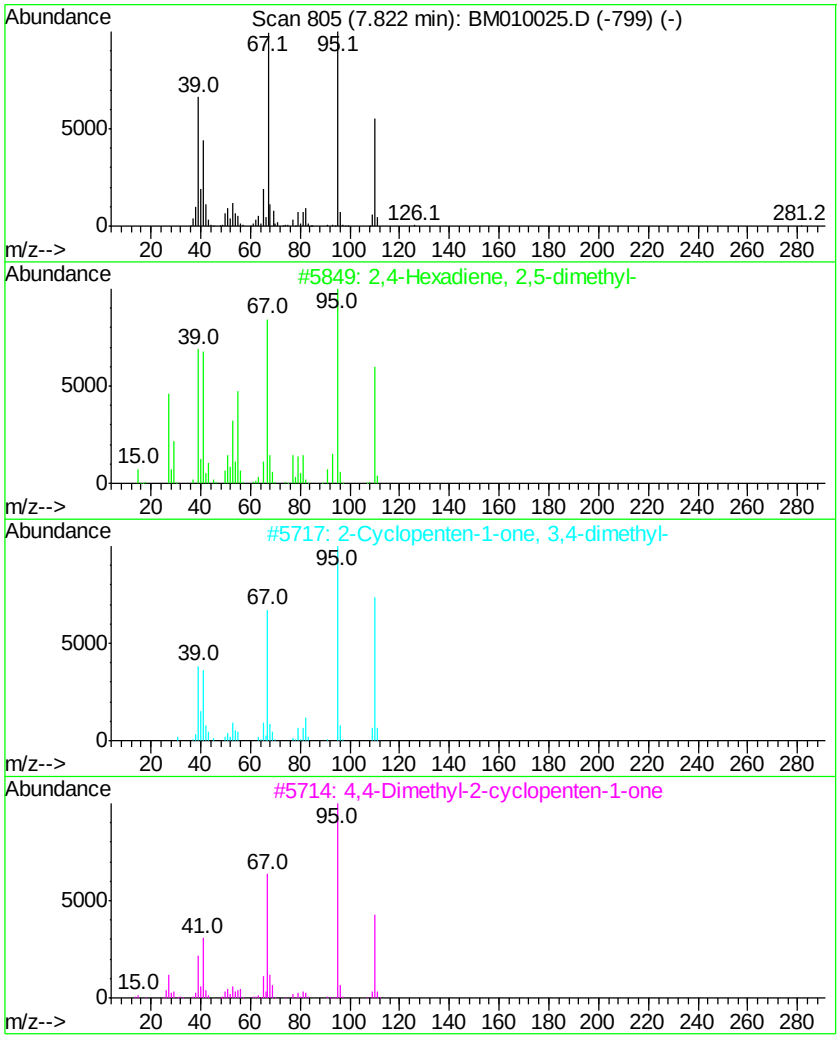
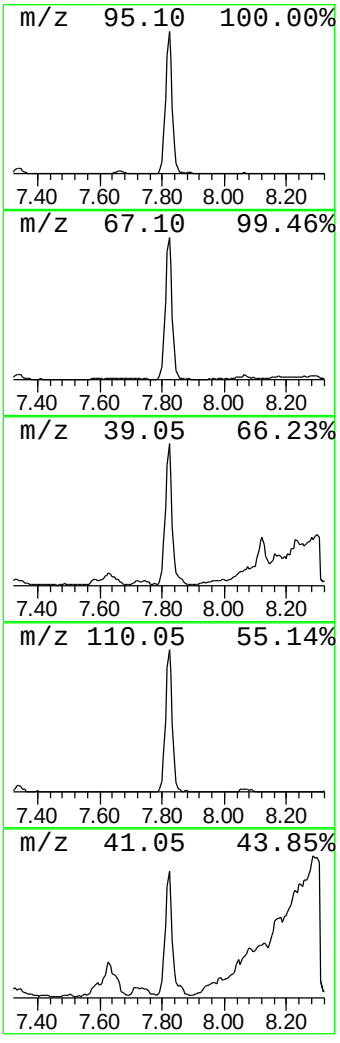
Peak Number 11 2,4-Hexadiene, 2,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	104.40 ng	2357650	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	90
2	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	70
3	4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	64
4	1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	50
5	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	49





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Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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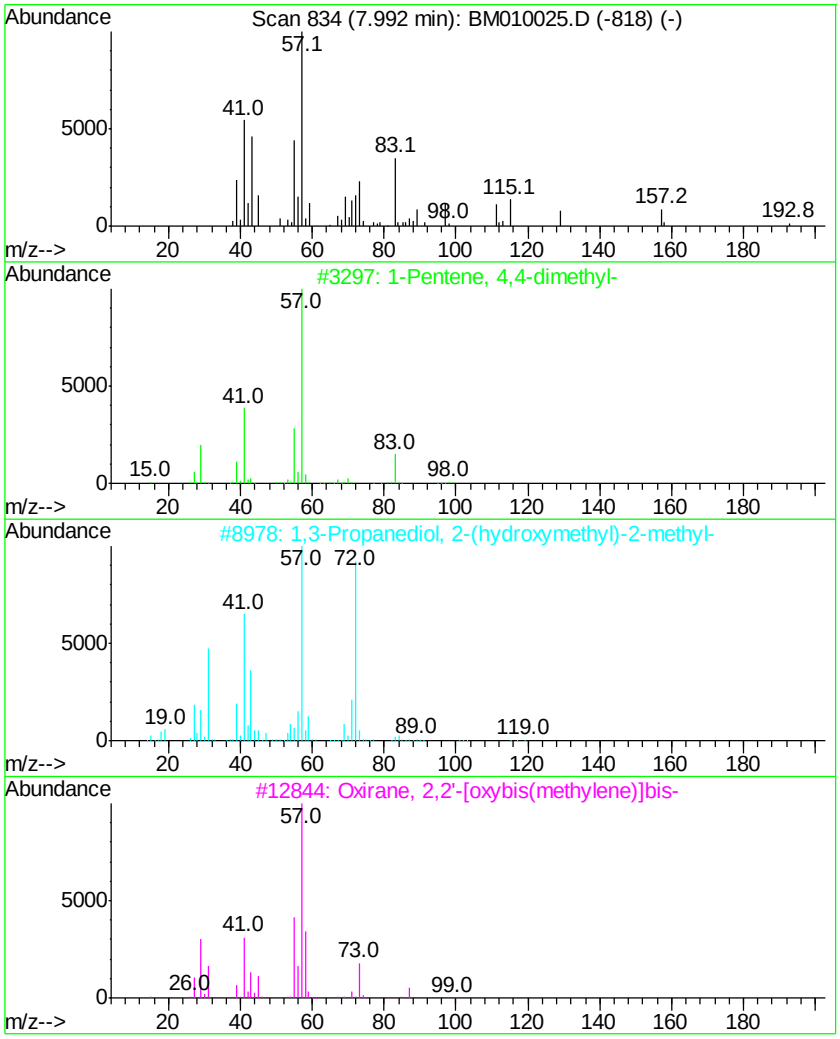
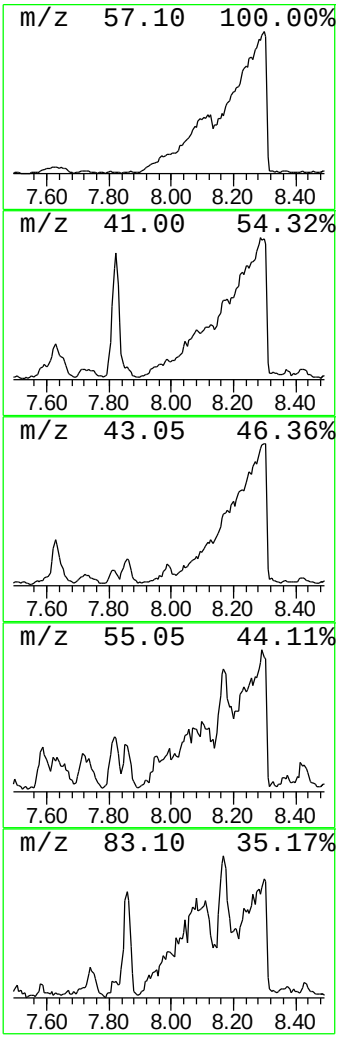
Peak Number 12 unknown7.99 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.99	21.50 ng	485490	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	22
2	1,3-Propanediol, 2-(hydroxymethy...	120	C5H12O3	000077-85-0	14
3	Oxirane, 2,2'-[oxybis(methylene)...	130	C6H10O3	002238-07-5	14
4	1-ISOBUTOXY-1-METHOXYPROPANE	146	C8H18O2	1000245-16-6	10
5	Oxirane, (3,3-dimethylbutyl)-	128	C8H16O	053907-77-0	10





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Instrument : BNA_M
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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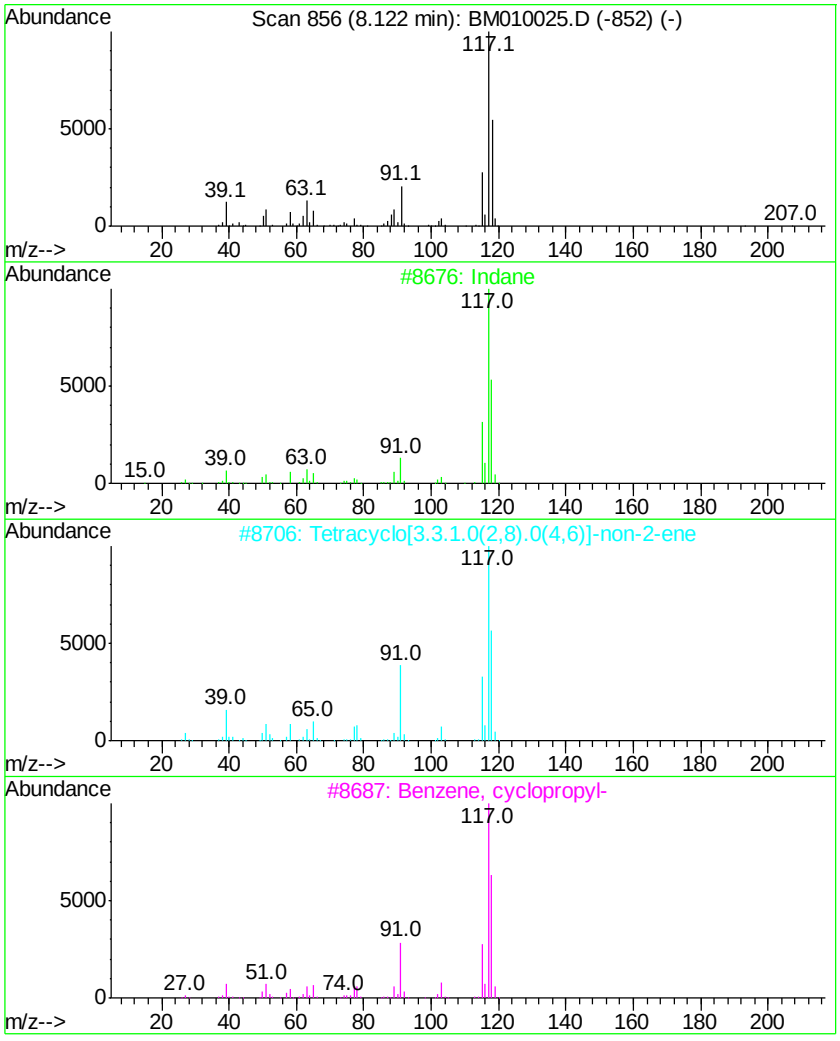
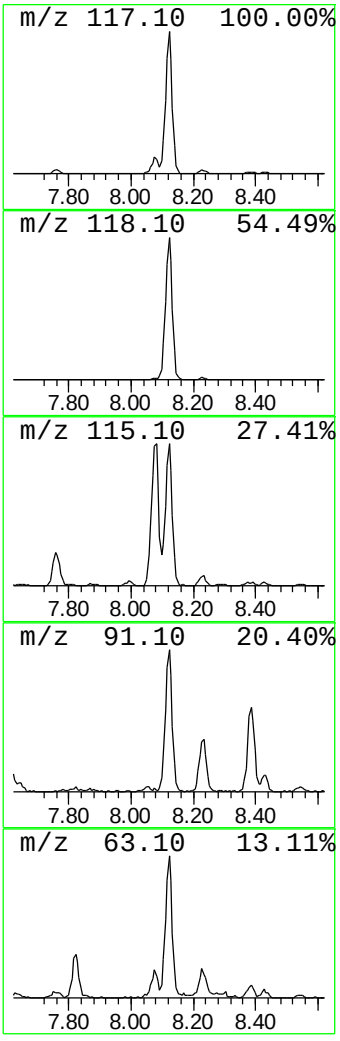
Peak Number 14 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.12	56.06 ng	1265950	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	81
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Deltacyclene	118	C9H10	007785-10-6	58
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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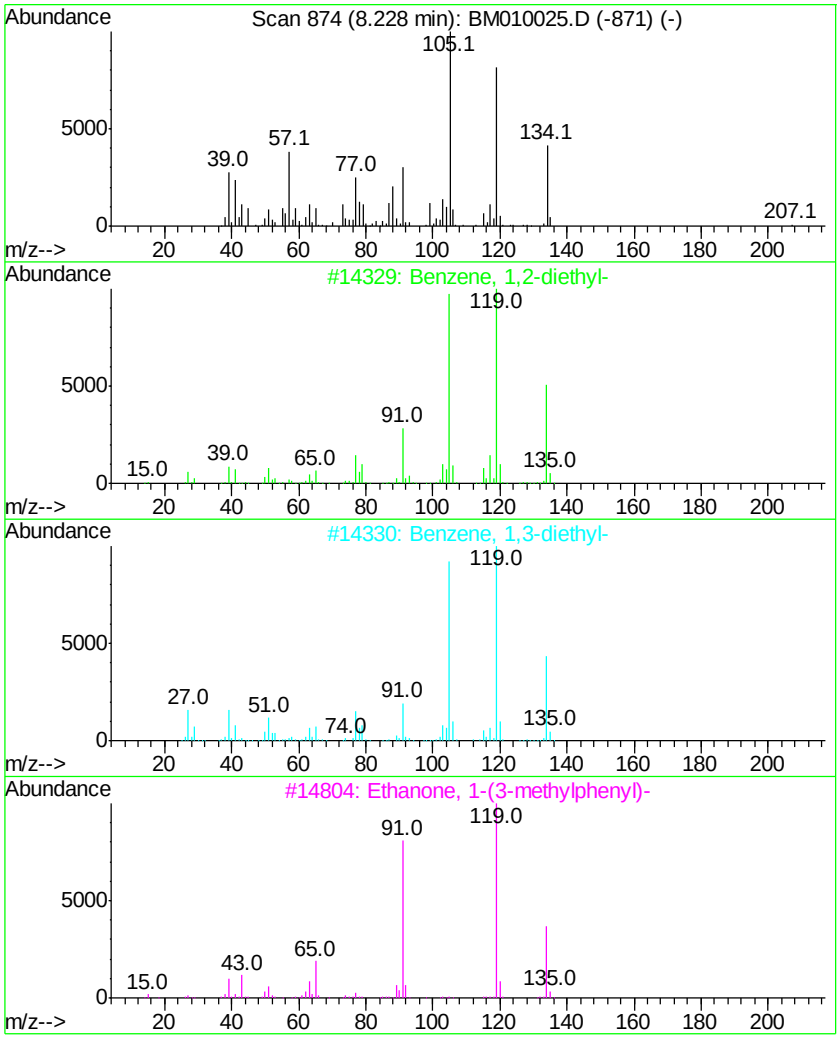
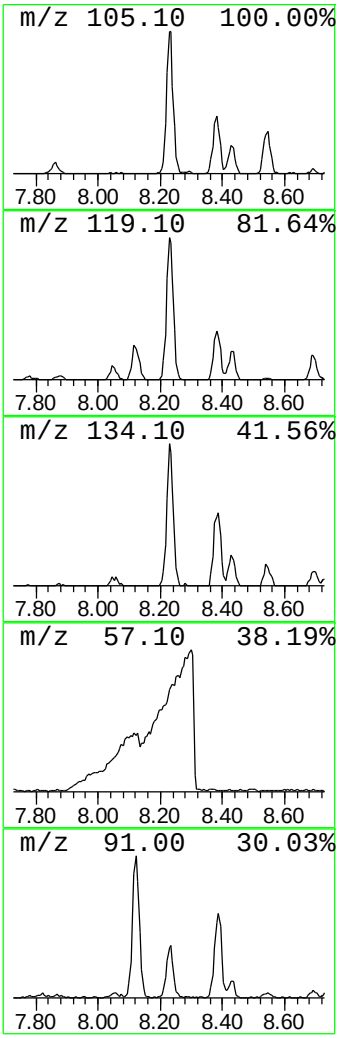
Peak Number 15 Benzene, 1,2-diethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	34.53 ng	779864	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
2	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
3	Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	87
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	81
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	74





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Instrument : BNA_M
ClientSampleId : MW-1R

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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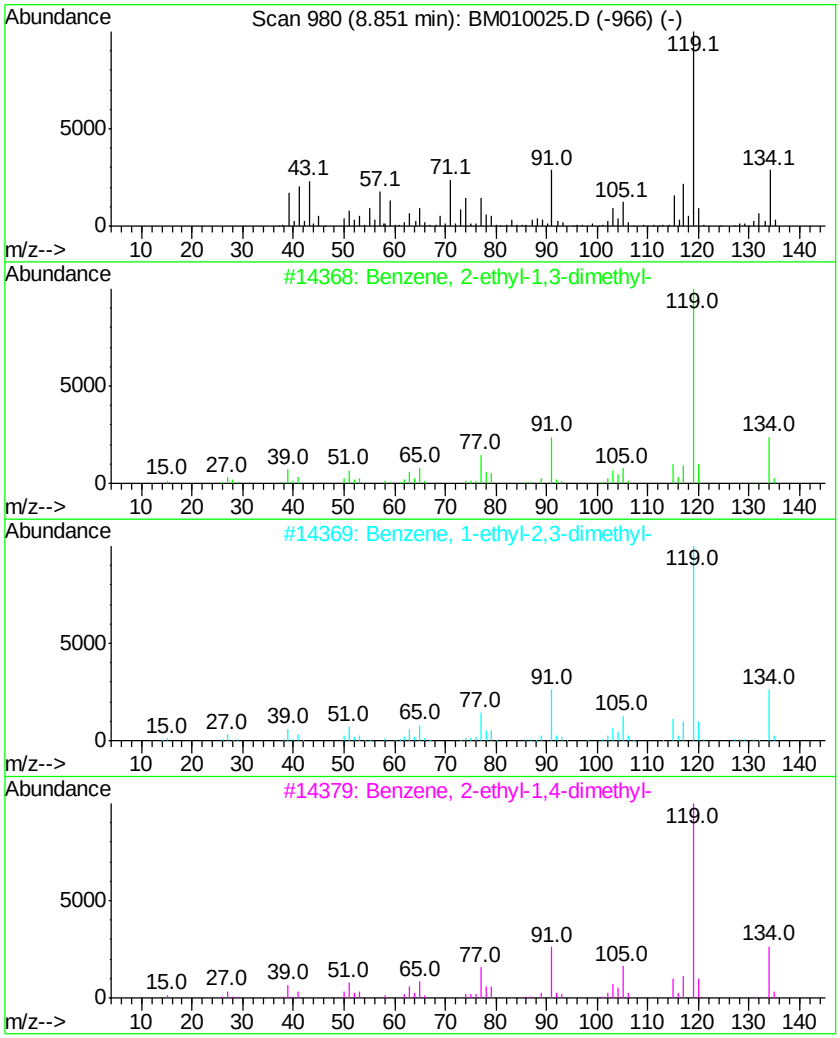
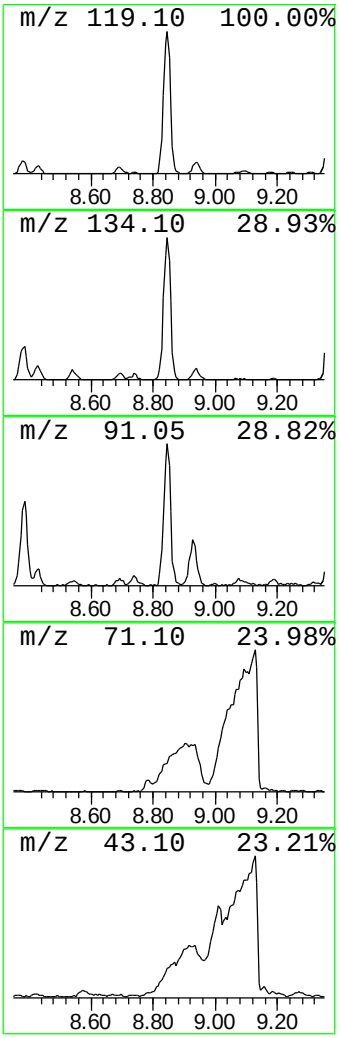
Peak Number 16 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	98.24 ng	2218480	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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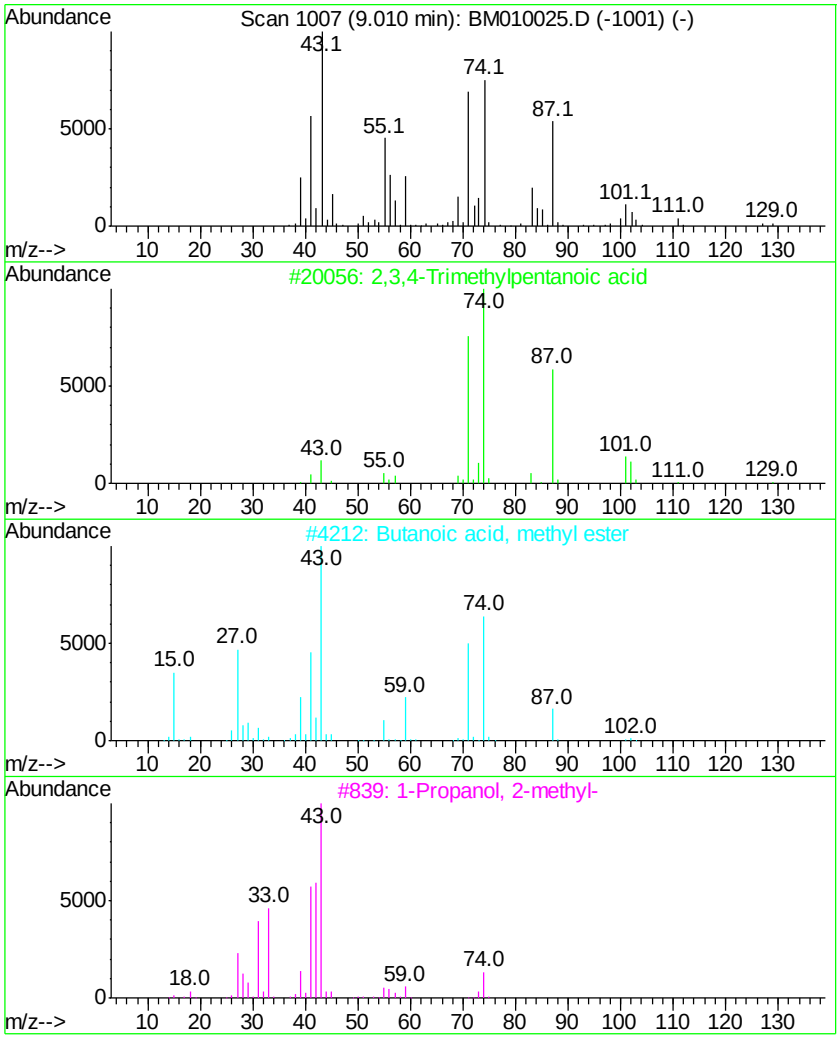
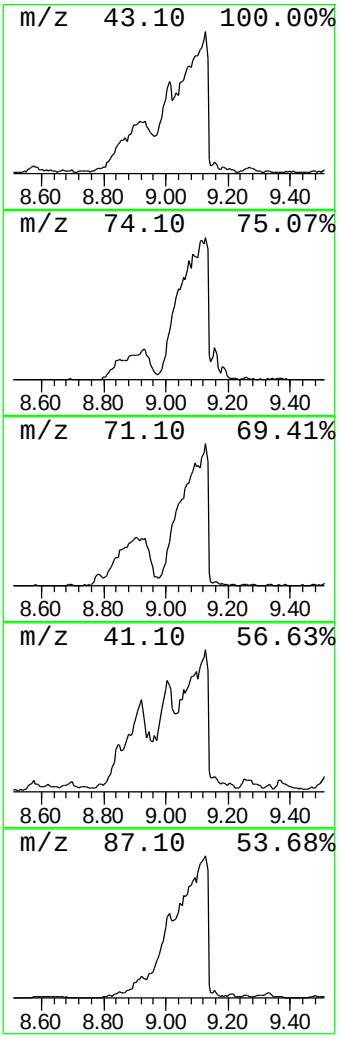
Peak Number 17 2,3,4-Trimethylpentanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	42.10 ng	950749	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,4-Trimethylpentanoic acid	144	C8H16O2	090435-18-0	53
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	43
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
4	2-O-Methyl-d-xylose	164	C6H12O5	1000130-01-3	27
5	Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	27





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Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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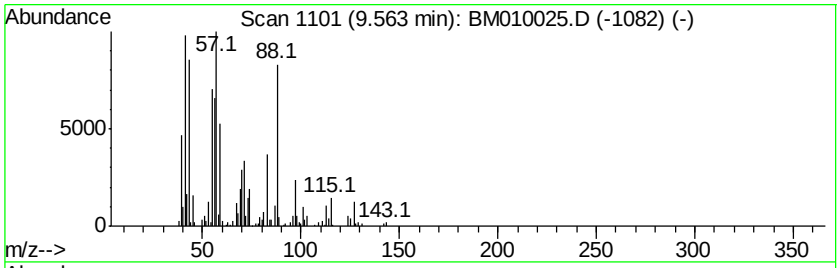
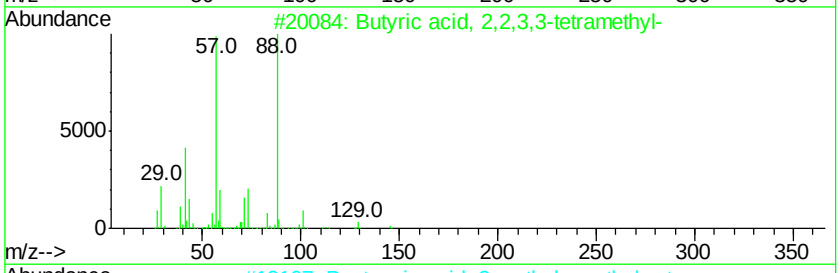
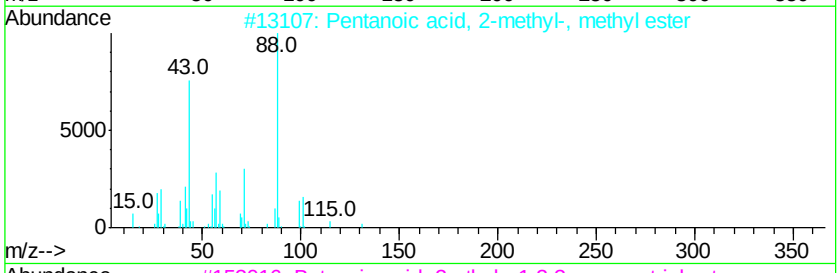
Peak Number 18 unknown9.56 Concentration Rank 11

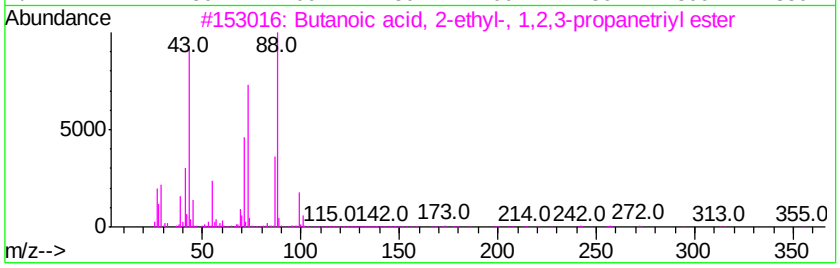
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.56	35.17 ng	1426980	Naphthalene-d8	10.55

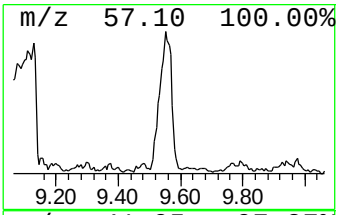
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	47
2	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	47
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38
4	2-Amino-2-ethyl-1,3-propanediol	119	C5H13NO2	000115-70-8	38
5	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	38

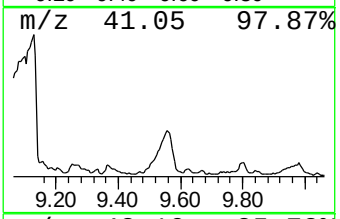


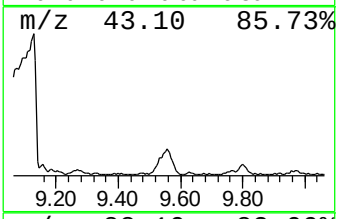


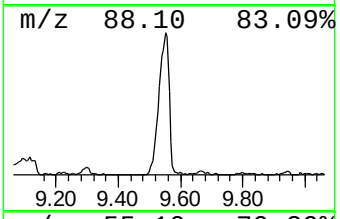


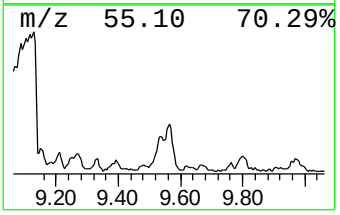












Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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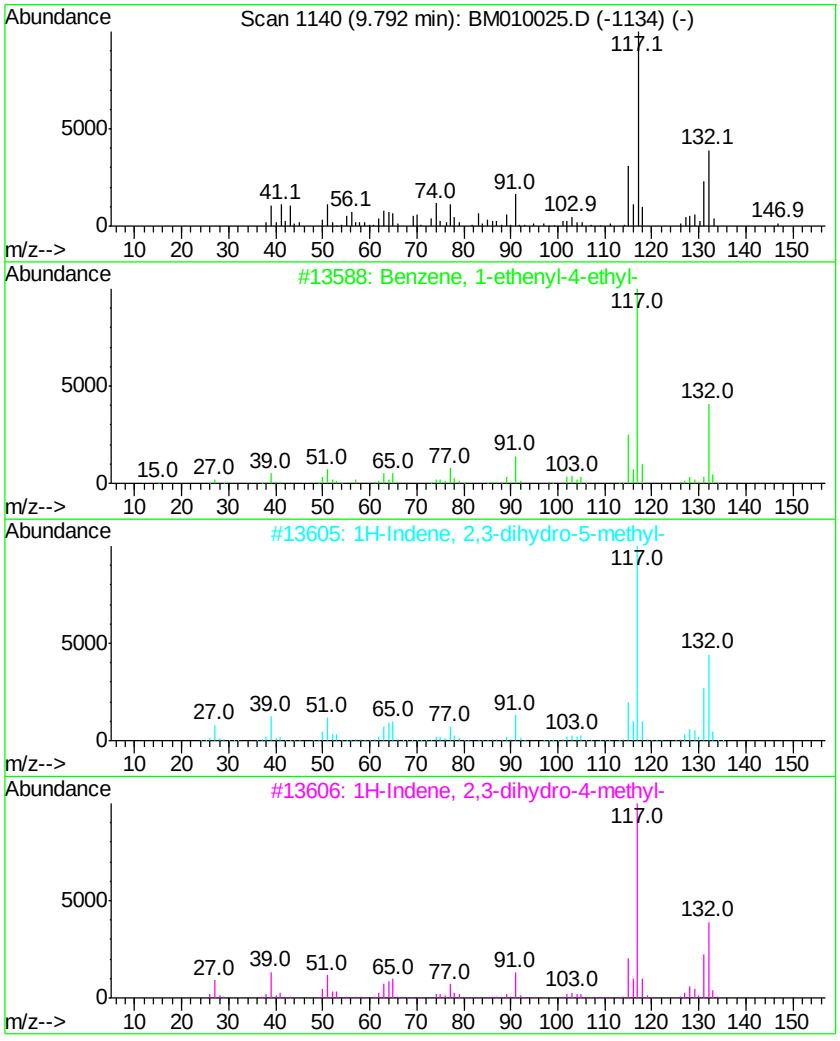
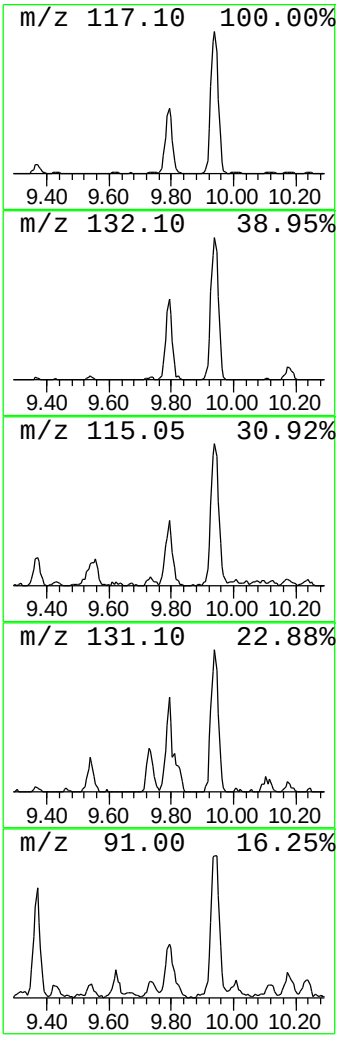
Peak Number 19 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	14.38 ng	583459	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

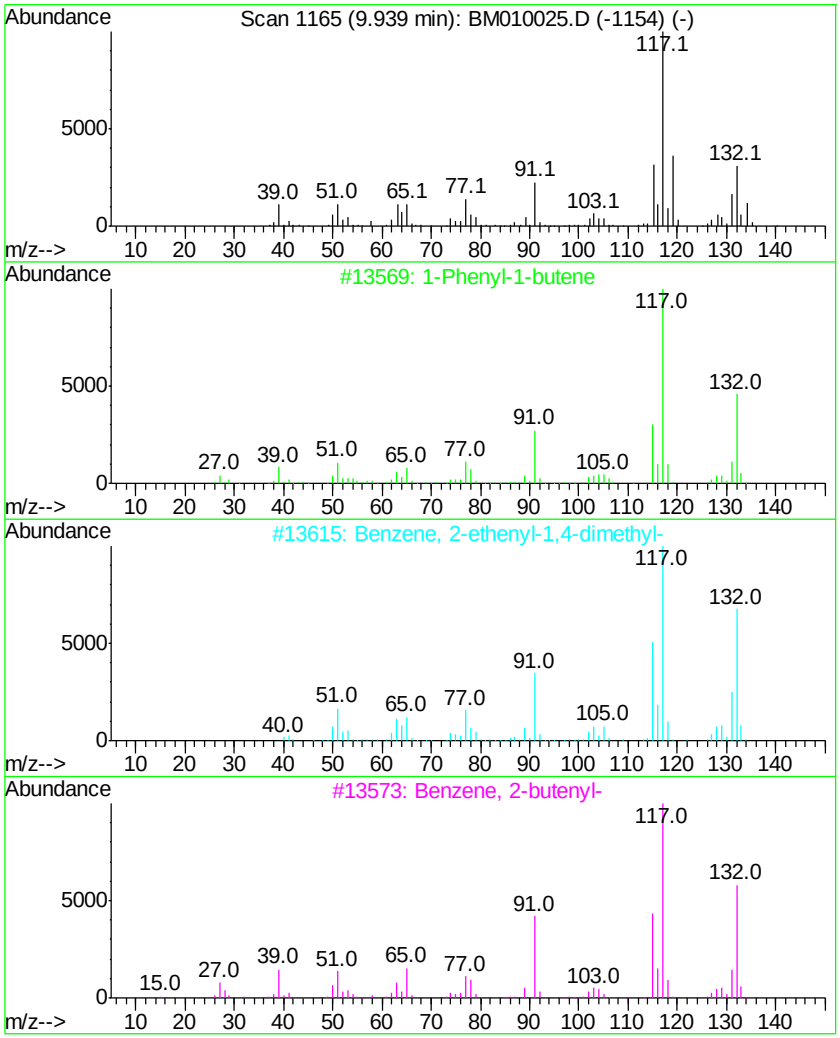
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

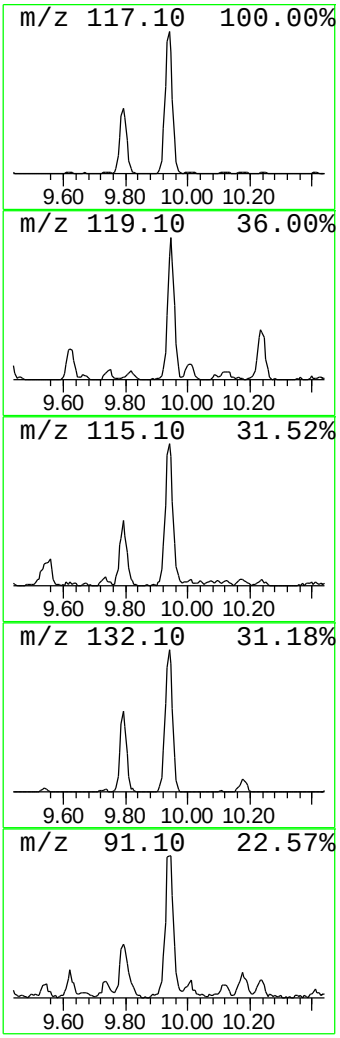
****

Peak Number 20 1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	37.28 ng	1512530	Naphthalene-d8	10.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051217\
Data File : BM010025.D
Acq On : 12 May 2017 16:03
Operator : SJ/MA
Sample : I3098-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-1R

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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
2-Butanol, 2,3-di...	3.51	15.8	ng	357071	1	7.76	451643	20.0
unknown4.29	4.29	28.1	ng	635184	1	7.76	451643	20.0
1,3-Dimethylcyclo...	4.98	24.8	ng	558929	1	7.76	451643	20.0
Cyclopentanone, 2...	5.66	32.9	ng	742026	1	7.76	451643	20.0
3,4-Dimethylcyclo...	6.05	78.2	ng	1766120	1	7.76	451643	20.0
trans-3,4-Dimethy...	6.52	103.6	ng	2339040	1	7.76	451643	20.0
Benzene, propyl-	6.73	14.7	ng	330728	1	7.76	451643	20.0
3-Ethylcyclopenta...	6.83	29.2	ng	659193	1	7.76	451643	20.0
3H-1,2-Dithiol-3-...	7.30	91.5	ng	2065240	1	7.76	451643	20.0
1-Hydroxy-4-hydra...	7.63	44.4	ng	1002190	1	7.76	451643	20.0
2,4-Hexadiene, 2,...	7.82	104.4	ng	2357650	1	7.76	451643	20.0
unknown7.99	7.99	21.5	ng	485490	1	7.76	451643	20.0
Indane	8.12	56.1	ng	1265950	1	7.76	451643	20.0
Benzene, 1,2-diet...	8.23	34.5	ng	779864	1	7.76	451643	20.0
Benzene, 2-ethyl-...	8.85	98.2	ng	2218480	1	7.76	451643	20.0
2,3,4-Trimethylpe...	9.01	42.1	ng	950749	1	7.76	451643	20.0
unknown9.56	9.56	35.2	ng	1426980	2	10.55	811438	20.0
Benzene, 1-etheny...	9.79	14.4	ng	583459	2	10.55	811438	20.0
1-Phenyl-1-butene	9.94	37.3	ng	1512530	2	10.55	811438	20.0