LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

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_G\METHODS\8270-BG122117.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	3.449	18	27	38	rBV	77616	172720	3.63%	0.285%
2	4.718	236	243	249	rBV	135996	238348	5.00%	0.394%
3	6.187	482	493	498	rBV	1151005	2031504	42.64%	3.355%
4	6.240	498	502	510	rVV	320451	572096	12.01%	0.945%
5	6.352	510	521	537	rVB	1745174	3378708	70.92%	5.579%
6	6.728	577	585	599	rVB	1053198	1849853	38.83%	3.055%
7	7.239	665	672	680	rBV	156532	276190	5.80%	0.456%
8	7.750	752	759	768	rBV	177655	323591	6.79%	0.534%
9	7.867	773	779	783	rVV	222417	388007	8.14%	0.641%
10	7.926	783	789	796	rVV2	716398	1347676	28.29%	2.225%
11	8.008	796	803	814	rVB	896060	1564963	32.85%	2.584%
12	8.185	823	833	845	rBV	404255	768321	16.13%	1.269%
13	8.338	851	859	867	rVB	642541	1177851	24.72%	1.945%
14	8.461	867	880	890	rBV	2342892	4305483	90.37%	7.110%
15	8.825	936	942	945	rBV	140053	258622	5.43%	0.427%
16	8.943	953	962	970	rBV	860045	1577008	33.10%	2.604%
17	9.066	970	983	986	rBV3	61266	158136	3.32%	0.261%
18	9.166	992	1000	1004	rBV	628148	1202156	25.23%	1.985%
19	9.219	1004	1009	1020	rVB	408125	765557	16.07%	1.264%
20	9.325	1021	1027	1032	rBV2	99229	173276	3.64%	0.286%
21	9.383	1032	1037	1045	rVB	200356	345101	7.24%	0.570%
22	9.471	1045	1052	1059	rBV2	420185	797344	16.74%	1.317%
23	9.530	1059	1062	1067	rVB2	44709	69698	1.46%	0.115%
24	9.648	1076	1082	1089	rBV2	135484	271099	5.69%	0.448%
25	9.800	1102	1108	1113	rBV	229100	395579	8.30%	0.653%
26	9.853	1113	1117	1128	rVB	244236	471998	9.91%	0.779%
27	9.959	1128	1135	1141	rBV2	377018	718674	15.08%	1.187%
28	10.030	1141	1147	1160	rVB3	484843	1349203	28.32%	2.228%
29	10.212	1167	1178	1187	rBV6	84516	254226	5.34%	0.420%
30	10.306	1187	1194	1199	rBV2	129053	253783	5.33%	0.419%
31	10.494	1220	1226	1231	rBV	272501	473788	9.94%	0.782%
32	10.558	1231	1237	1243	rVB	406206	698950	14.67%	1.154%
33	10.752	1262	1270	1274	rBV5	27343	85485	1.79%	0.141%
34	10.870	1283	1290	1297	rVV4	133436	321777	6.75%	0.531%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

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_G\METHODS\8270-BG122117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.934	1297	1301	1310	rVB2	135939	253210	5.31%	0.418%
36	11.093	1320	1328	1334	rBV	692742	1318556	27.68%	2.177%
37	11.146	1334	1337	1347	rVB4	80501	167751	3.52%	0.277%
38	11.334	1363	1369	1375	rBV	271158	533176	11.19%	0.880%
39	11.381	1375	1377	1385	rVB	63550	87556	1.84%	0.145%
40	11.569	1398	1409	1412	rBV5	34707	96523	2.03%	0.159%
41	11.610	1412	1416	1419	rBV3	40085	69456	1.46%	0.115%
42	11.681	1424	1428	1430	rVV2	71601	110010	2.31%	0.182%
43	11.716	1430	1434	1437	rVV	187374	335935	7.05%	0.555%
44	11.769	1437	1443	1449	rVB	1028349	1941792	40.76%	3.207%
45	11.904	1459	1466	1471	rBV4	55658	113619	2.38%	0.188%
46	12.063	1488	1493	1497	rBV2	52314	97761	2.05%	0.161%
47	12.168	1505	1511	1520	rVV2	152970	289623	6.08%	0.478%
48	12.280	1520	1530	1539	rBV3	73112	196622	4.13%	0.325%
49	12.362	1539	1544	1555	rVB8	74625	206005	4.32%	0.340%
50	12.591	1580	1583	1592	rVB4	69316	120370	2.53%	0.199%
51	12.779	1611	1615	1620	rVB	58804	93671	1.97%	0.155%
52	12.867	1625	1630	1640	rVB3	197977	376624	7.91%	0.622%
53	12.985	1646	1650	1656	rBV	38491	73144	1.54%	0.121%
54	13.044	1656	1660	1672	rVB4	186985	392381	8.24%	0.648%
55	13.208	1684	1688	1695	rVB	142709	242631	5.09%	0.401%
56	13.326	1702	1708	1713	rBV	960582	1566181	32.87%	2.586%
57	13.373	1713	1716	1725	rVB3	77319	131508	2.76%	0.217%
58	13.461	1725	1731	1736	rBV3	96098	230268	4.83%	0.380%
59	13.537	1737	1744	1755	rBV2	872798	2207132	46.33%	3.645%
60	13.808	1785	1790	1795	rVB3	112920	177081	3.72%	0.292%
61	13.860	1796	1799	1805	rVB6	50512	80720	1.69%	0.133%
62	13.931	1805	1811	1814	rBV4	51467	106160	2.23%	0.175%
63	14.090	1831	1838	1844	rBV	1766887	2778581	58.32%	4.588%
64	14.148	1844	1848	1851	rVV2	92328	172548	3.62%	0.285%
65	14.178	1851	1853	1862	rVB4	135665	250979	5.27%	0.414%
66	14.283	1862	1871	1886	rBV3	210001	640530	13.44%	1.058%
67	14.407	1887	1892	1894	rBV4	45476	81347	1.71%	0.134%
68	14.495	1902	1907	1910	rBV3	82205	135388	2.84%	0.224%
69	14.630	1924	1930	1936	rBV4	260695	723802	15.19%	1.195%
70	14.777	1950	1955	1960	rVV2	242194	456994	9.59%	0.755%
71	14.836	1960	1965	1972	rVB3	256620	457854	9.61%	0.756%

LSC Area Percent Report

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Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

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_G\METHODS\8270-BG122117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	15.012	1989	1995	1999	rBV3	90346	178038	3.74%	0.294%
73	15.059	1999	2003	2011	rVB7	106348	209262	4.39%	0.346%
74	15.182	2019	2024	2028	rVB4	64351	114811	2.41%	0.190%
75	15.241	2028	2034	2041	rVB3	119558	223105	4.68%	0.368%
76	15.370	2051	2056	2059	rBV3	54708	83548	1.75%	0.138%
77	15.417	2060	2064	2066	rBV2	66971	97510	2.05%	0.161%
78	15.459	2066	2071	2077	rVB2	367139	600956	12.61%	0.992%
79	15.564	2085	2089	2092	rBV5	100951	173806	3.65%	0.287%
80	15.688	2107	2110	2115	rVB2	82203	104703	2.20%	0.173%
81	15.741	2115	2119	2124	rBV7	42362	95755	2.01%	0.158%
82	15.793	2125	2128	2132	rVV3	75726	109687	2.30%	0.181%
83	15.840	2133	2136	2142	rVB3	72701	109965	2.31%	0.182%
84	15.923	2142	2150	2164	rBV4	117544	415769	8.73%	0.687%
85	16.064	2167	2174	2179	rBV5	169322	362443	7.61%	0.599%
86	16.158	2185	2190	2193	rBV6	42937	87268	1.83%	0.144%
87	16.199	2193	2197	2202	rVB8	76502	131810	2.77%	0.218%
88	16.299	2212	2214	2220	rVB5	56921	89790	1.88%	0.148%
89	16.469	2238	2243	2246	rBV6	59981	108155	2.27%	0.179%
90	16.763	2289	2293	2298	rVB6	59109	97842	2.05%	0.162%
91	16.933	2316	2322	2331	rVB	1435961	2340346	49.12%	3.865%
92	17.345	2388	2392	2397	rVB6	40061	72006	1.51%	0.119%
93	17.533	2419	2424	2428	rBV3	88724	151234	3.17%	0.250%
94	18.197	2531	2537	2550	rVB	521015	917015	19.25%	1.514%
95	18.649	2610	2614	2621	rVB9	33963	67401	1.41%	0.111%
96	19.013	2672	2676	2681	rBV2	112409	152693	3.21%	0.252%
97	20.253	2882	2887	2896	rBV	129858	195859	4.11%	0.323%
98	20.729	2961	2968	2976	rBV	3371747	4764168	100.00%	7.867%
99	22.550	3271	3278	3287	rVB2	564199	1058515	22.22%	1.748%
100	26.340	3911	3923	3938	rBV2	326707	1093933	22.96%	1.806%

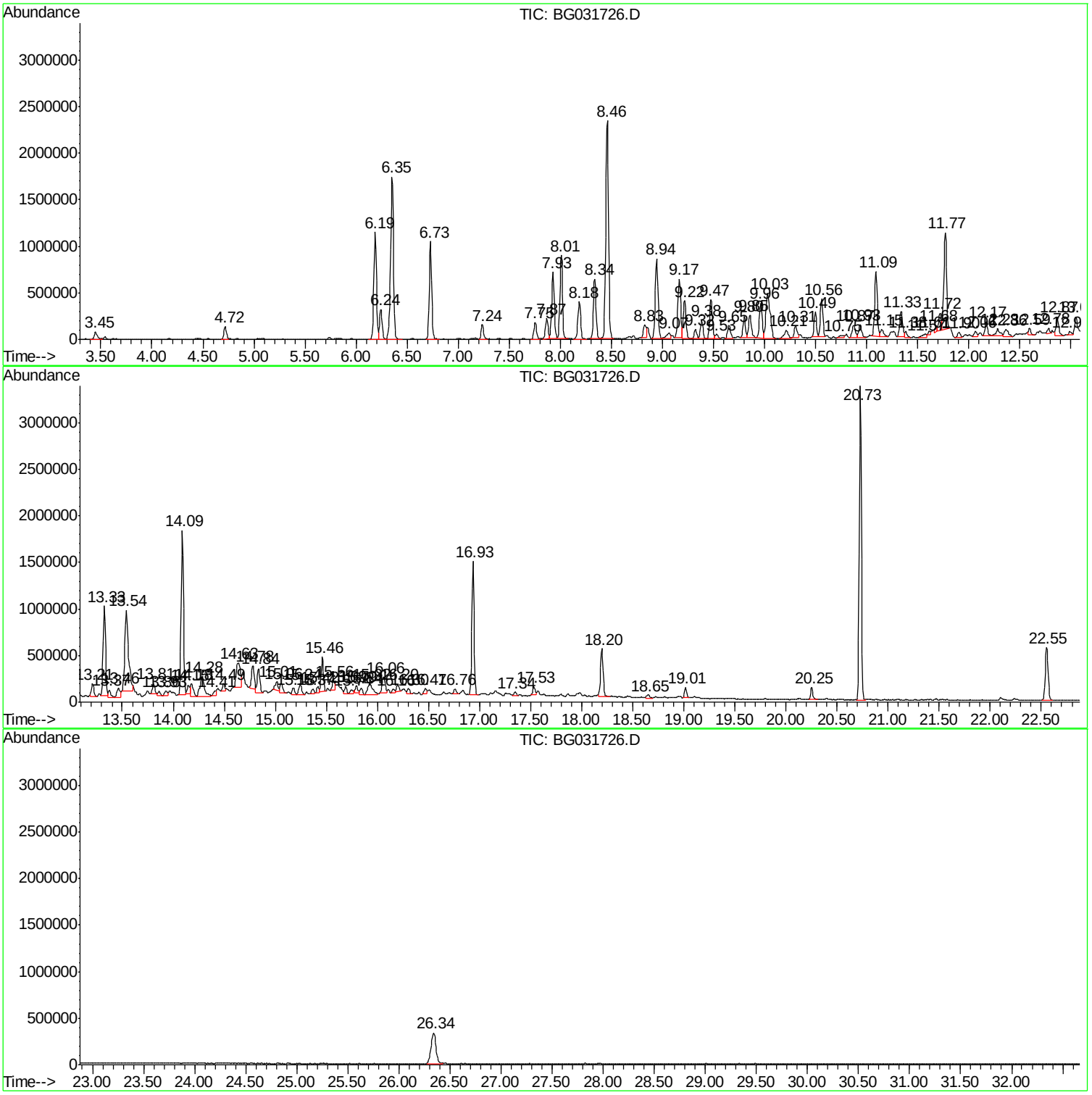
Sum of corrected areas: 60557653

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

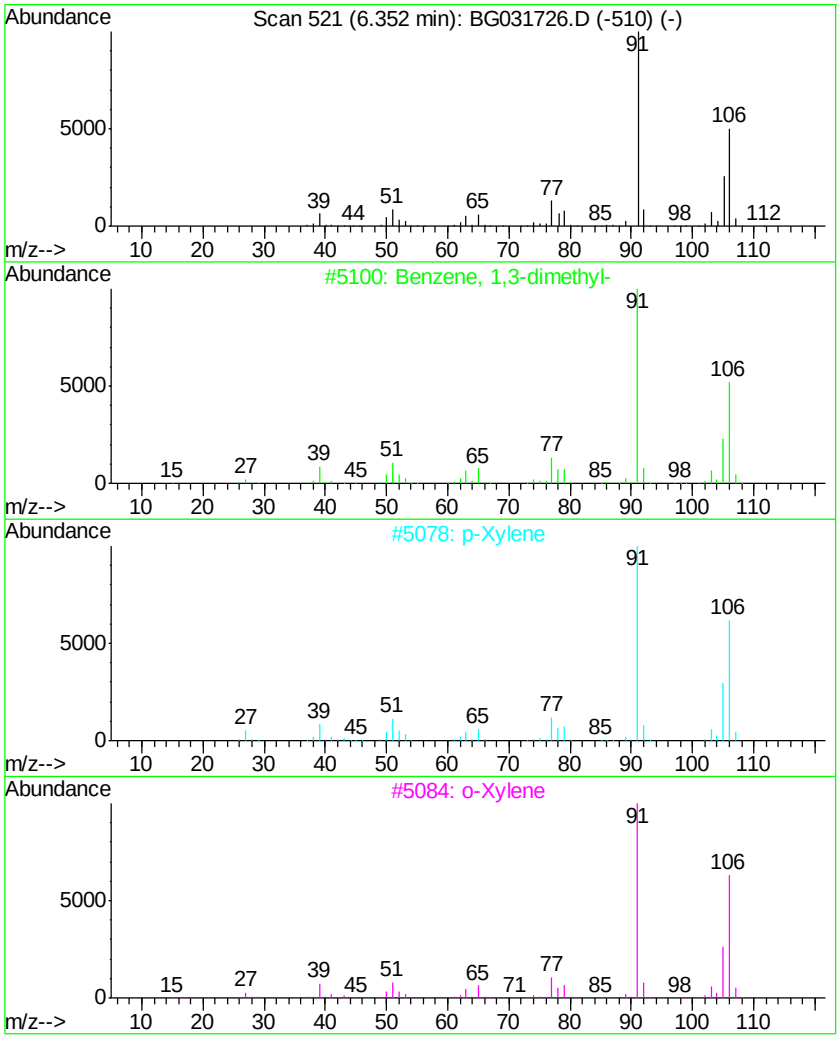
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

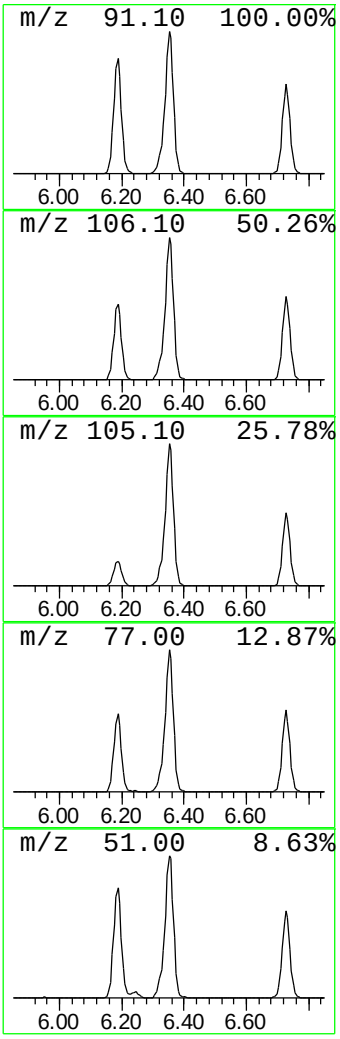
****

Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	261.29 ng	3378710	1,4-Dichlorobenzene-d4	8.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2	p-Xylene	106	C8H10	000106-42-3	97
3	o-Xylene	106	C8H10	000095-47-6	95
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87
5	Ethylbenzene	106	C8H10	000100-41-4	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

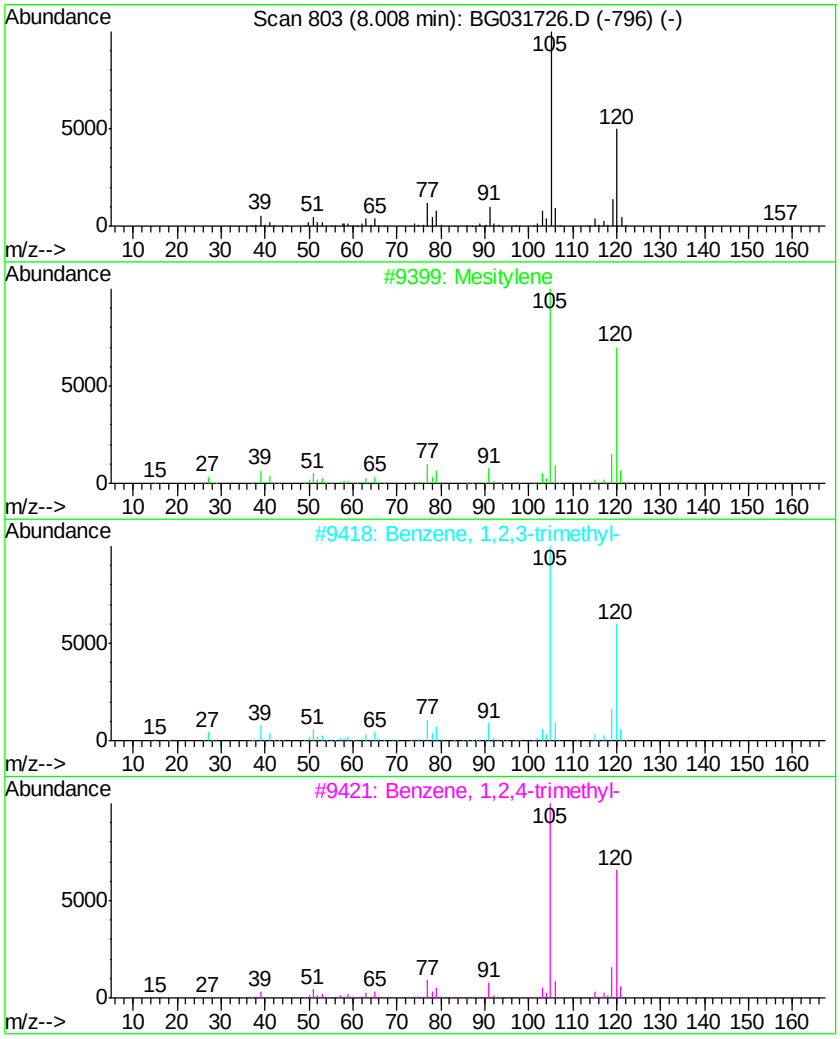
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

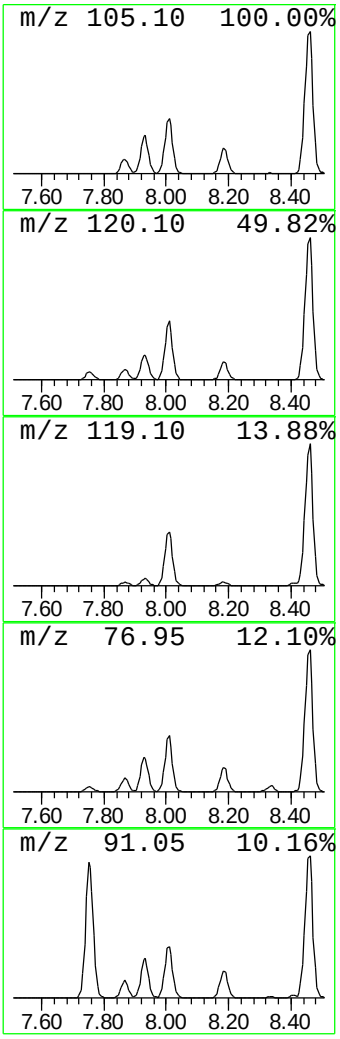
****

Peak Number 4 Mesitylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	121.02 ng	1564960	1,4-Dichlorobenzene-d4	8.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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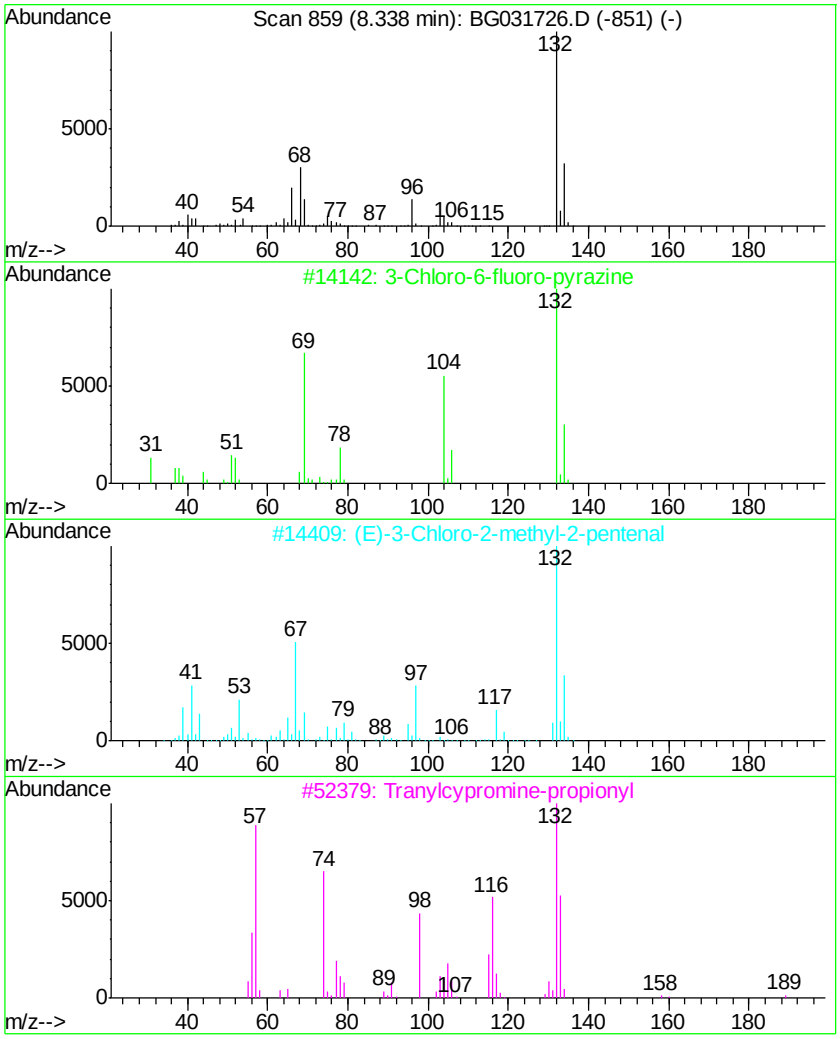
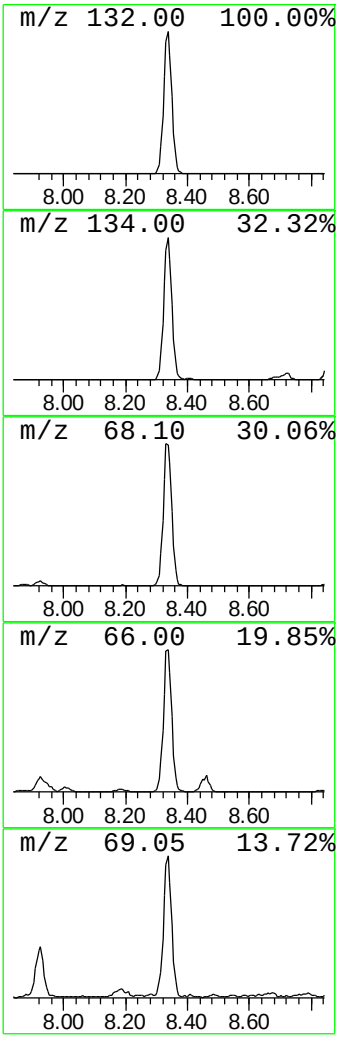
Peak Number 5 unknown8.34 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	91.09 ng	1177850	1,4-Dichlorobenzene-d4	8.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

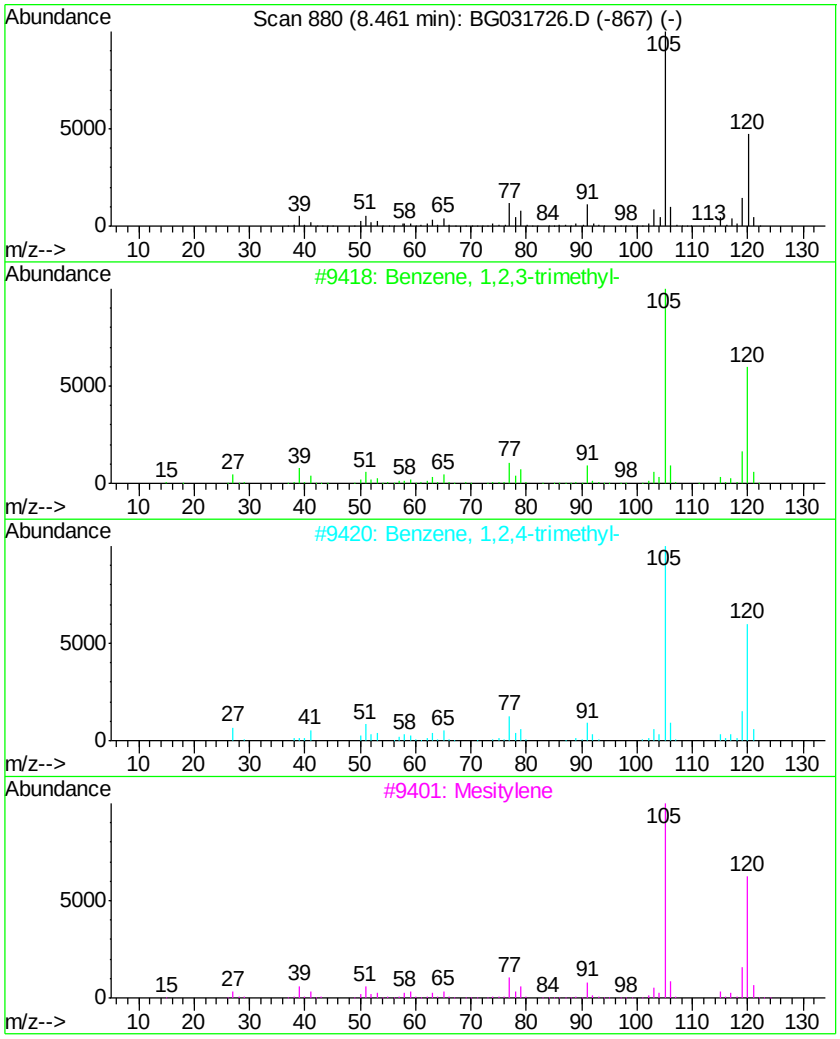
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

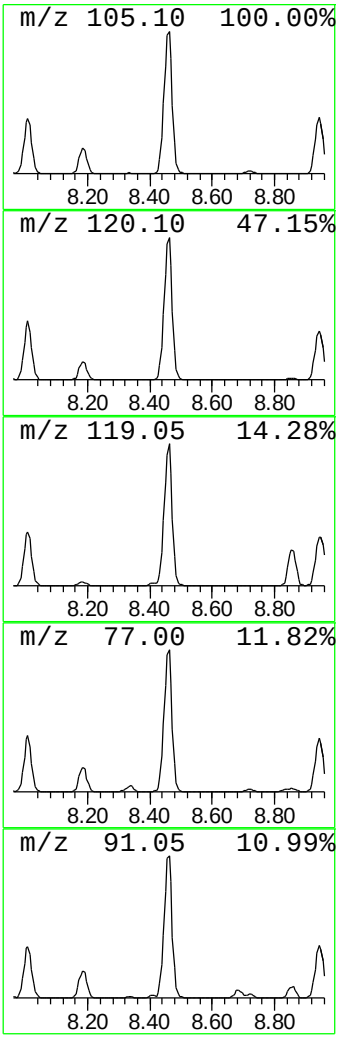
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	332.96 ng	4305480	1,4-Dichlorobenzene-d4	8.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

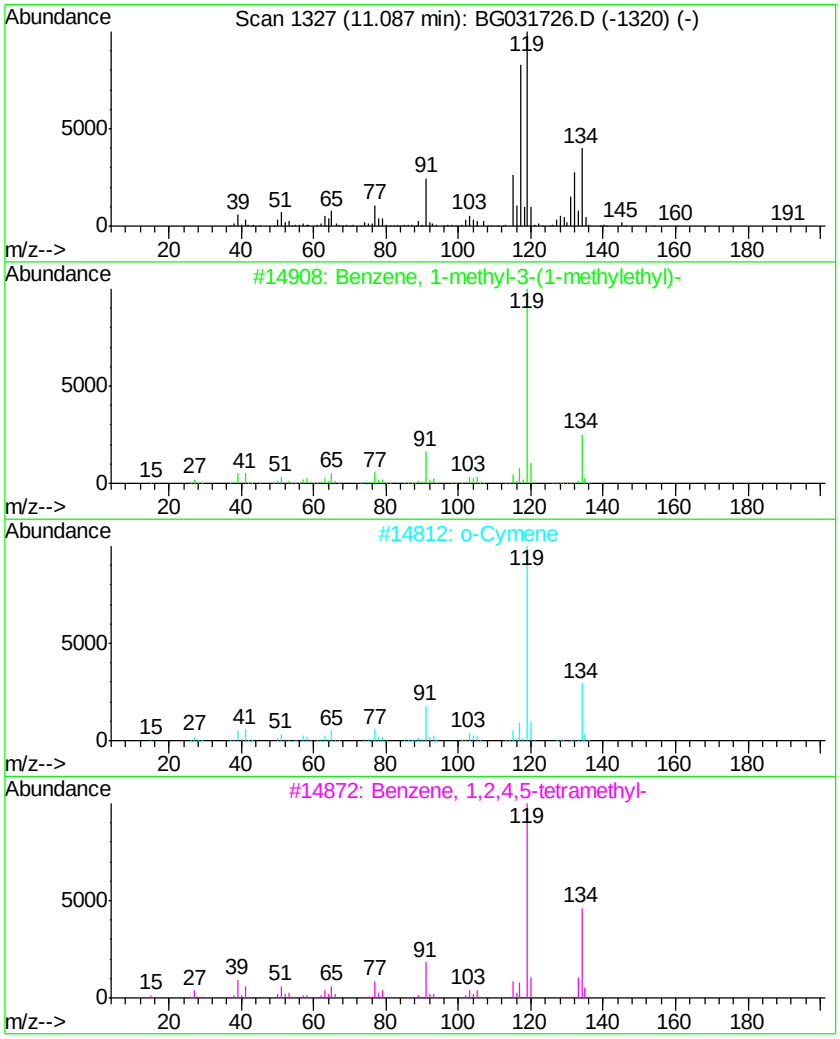
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

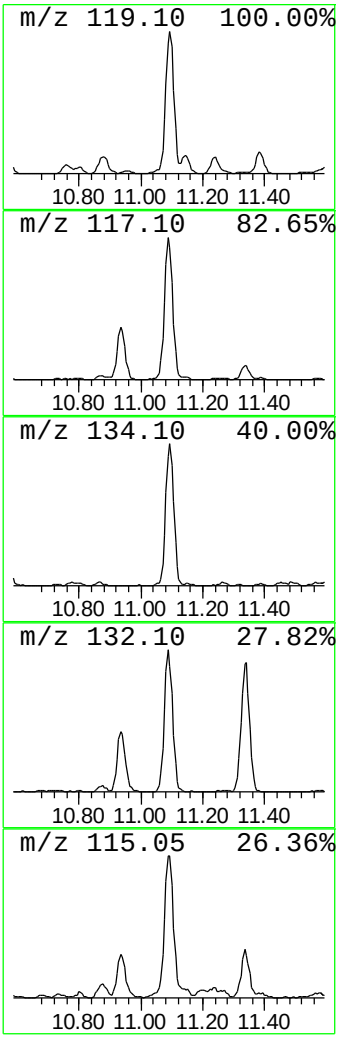
****

Peak Number 9 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	78.50 ng	1318560	Naphthalene-d8	11.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60
2	o-Cymene	134	C10H14	000527-84-4	60
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	60
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	53
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	53





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

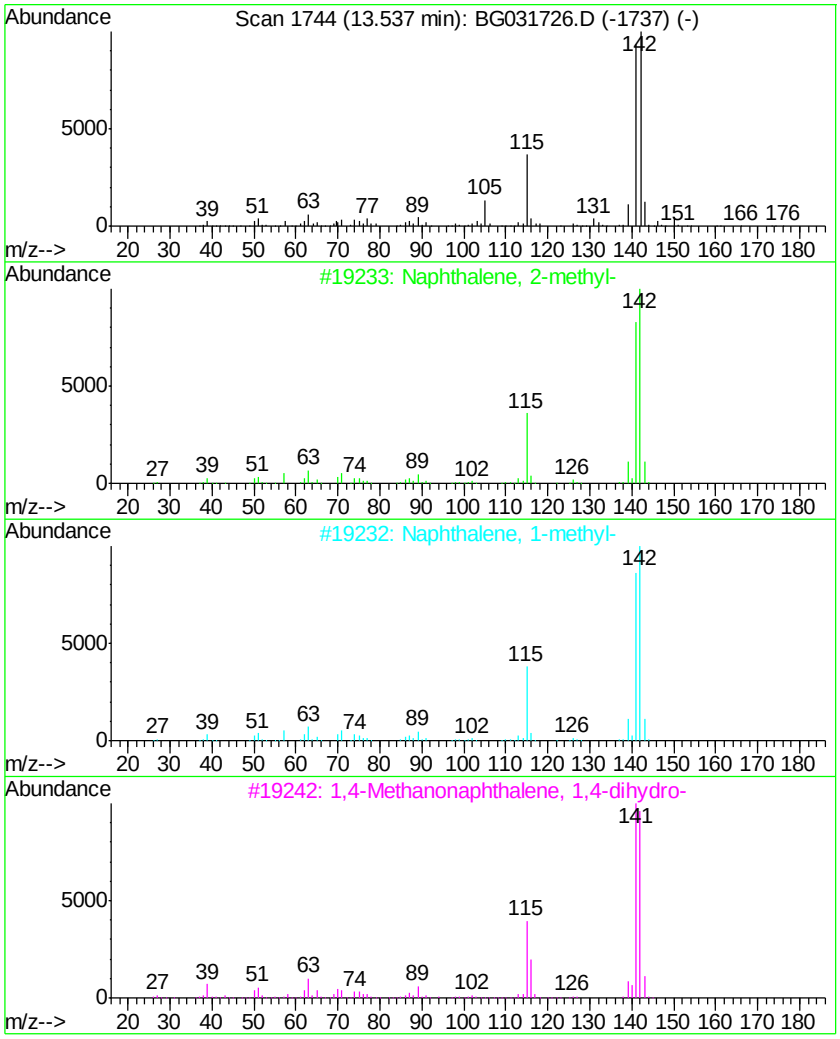
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

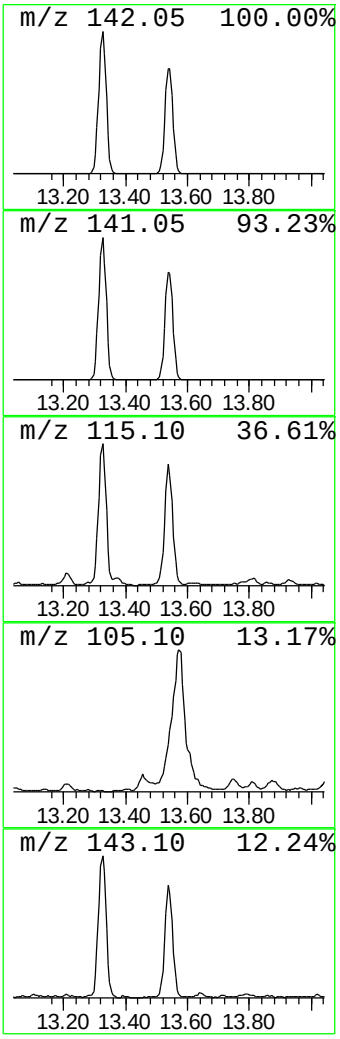
****

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	131.40 ng	2207130	Naphthalene-d8	11.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122217\
Data File : BG031726.D
Acq On : 23 Dec 2017 00:25
Operator : SJ/JU
Sample : I7004-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PR-MW-1-121817

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 1,3-dime...	6.35	261.3	ng	3378710	1	8.83	258622	20.0
Mesitylene	8.01	121.0	ng	1564960	1	8.83	258622	20.0
unknown8.34	8.34	91.1	ng	1177850	1	8.83	258622	20.0
Benzene, 1,2,3-tr...	8.46	333.0	ng	4305480	1	8.83	258622	20.0
Benzene, 1-methyl...	11.09	78.5	ng	1318560	2	11.72	335935	20.0
Naphthalene, 1-me...	13.54	131.4	ng	2207130	2	11.72	335935	20.0