LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060420\
Data File : BF120551.D
Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.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	1.952	8	11	22	rBV	1497094	1958370	100.00%	14.134%
2	2.034	23	25	40	rVB	144332	267919	13.68%	1.934%
3	3.852	329	334	340	rVB	18001	24615	1.26%	0.178%
4	5.440	600	604	615	rVB	281671	245710	12.55%	1.773%
5	5.657	637	641	648	rBV	65108	73532	3.75%	0.531%
6	6.457	773	777	782	rBV	259936	237543	12.13%	1.714%
7	6.540	788	791	798	rVB	23174	24264	1.24%	0.175%
8	6.657	807	811	816	rBV	135392	161023	8.22%	1.162%
9	6.698	816	818	828	rVB	73114	79156	4.04%	0.571%
10	6.828	836	840	843	rBV	1173332	950502	48.54%	6.860%
11	6.981	862	866	869	rBV	314908	242856	12.40%	1.753%
12	7.087	880	884	892	rBV	83681	88972	4.54%	0.642%
13	7.381	931	934	937	rVV	192443	157605	8.05%	1.137%
14	7.440	941	944	949	rBV2	54926	69500	3.55%	0.502%
15	7.487	949	952	957	rVB	61614	49889	2.55%	0.360%
16	7.657	978	981	983	rBV	52833	49120	2.51%	0.354%
17	7.681	983	985	992	rVB	255013	212462	10.85%	1.533%
18	7.863	1012	1016	1019	rBV	66564	69423	3.54%	0.501%
19	7.892	1019	1021	1022	rBV	31619	27156	1.39%	0.196%
20	7.910	1022	1024	1027	rVB	103195	80031	4.09%	0.578%
21	7.981	1032	1036	1040	rVB2	19102	21926	1.12%	0.158%
22	8.110	1054	1058	1061	rBV	1645839	1331388	67.98%	9.609%
23	8.322	1091	1094	1098	rVB	176890	141814	7.24%	1.023%
24	8.381	1101	1104	1110	rBV	219456	179087	9.14%	1.292%
25	8.563	1131	1135	1141	rVB2	19907	23392	1.19%	0.169%
26	8.816	1174	1178	1184	rVB2	83725	84634	4.32%	0.611%
27	8.881	1186	1189	1193	rBV	72167	55542	2.84%	0.401%
28	8.922	1193	1196	1199	rBV	48218	37836	1.93%	0.273%
29	8.992	1206	1208	1210	rBV	54105	46150	2.36%	0.333%
30	9.104	1224	1227	1230	rBV	92536	64645	3.30%	0.467%
31	9.181	1237	1240	1245	rVB	337958	295647	15.10%	2.134%
32	9.310	1259	1262	1265	rBV2	46364	41951	2.14%	0.303%
33	9.339	1265	1267	1272	rVB	38074	34432	1.76%	0.248%
34	9.481	1287	1291	1295	rVB3	30979	33947	1.73%	0.245%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060420\
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Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.528	1295	1299	1302	rBV3	14561	19806	1.01%	0.143%
36	9.575	1304	1307	1313	rVB2	60162	82721	4.22%	0.597%
37	9.728	1329	1333	1337	rBV	77160	69632	3.56%	0.503%
38	9.869	1353	1357	1360	rVB	1236842	1063937	54.33%	7.678%
39	10.410	1447	1449	1455	rVB2	18328	25672	1.31%	0.185%
40	10.651	1485	1490	1494	rBV	188580	163173	8.33%	1.178%
41	10.780	1508	1512	1518	rVB4	35592	43785	2.24%	0.316%
42	10.857	1518	1525	1527	rBV4	17451	25528	1.30%	0.184%
43	10.957	1539	1542	1545	rBV3	14022	19685	1.01%	0.142%
44	11.251	1590	1592	1596	rVB2	24345	21096	1.08%	0.152%
45	11.357	1606	1610	1612	rBV	1159606	1059291	54.09%	7.645%
46	11.375	1612	1613	1616	rVV	96159	68187	3.48%	0.492%
47	11.428	1620	1622	1625	rVB	45475	33594	1.72%	0.242%
48	11.469	1625	1629	1631	rBV4	22888	29328	1.50%	0.212%
49	11.592	1647	1650	1654	rBV4	23298	27540	1.41%	0.199%
50	11.763	1676	1679	1683	rVB3	19651	28234	1.44%	0.204%
51	11.857	1692	1695	1697	rBV	55424	52912	2.70%	0.382%
52	11.886	1697	1700	1703	rVB2	54159	53944	2.75%	0.389%
53	11.963	1710	1713	1716	rBV2	65049	71507	3.65%	0.516%
54	11.992	1716	1718	1722	rVB2	46339	44157	2.25%	0.319%
55	12.027	1722	1724	1727	rBV2	20544	25010	1.28%	0.180%
56	12.122	1737	1740	1742	rBV2	18523	22856	1.17%	0.165%
57	12.151	1742	1745	1747	rVV2	40423	39418	2.01%	0.284%
58	12.175	1747	1749	1753	rVB4	17948	23401	1.19%	0.169%
59	12.333	1773	1776	1778	rBV	27370	27466	1.40%	0.198%
60	12.404	1785	1788	1791	rBV	72301	69396	3.54%	0.501%
61	12.439	1791	1794	1797	rVV3	39732	50523	2.58%	0.365%
62	12.492	1800	1803	1807	rBV3	41717	54801	2.80%	0.395%
63	12.569	1813	1816	1819	rVB	148570	124175	6.34%	0.896%
64	12.663	1829	1832	1834	rVB3	27635	22039	1.13%	0.159%
65	12.798	1851	1855	1857	rBV	270514	242350	12.38%	1.749%
66	12.857	1862	1865	1868	rVB	35658	37631	1.92%	0.272%
67	12.939	1876	1879	1882	rBV	292009	254087	12.97%	1.834%
68	13.016	1889	1892	1896	rBV2	42167	64691	3.30%	0.467%
69	13.121	1904	1910	1913	rBV3	51294	87414	4.46%	0.631%
70	13.227	1926	1928	1933	rBV	60823	64676	3.30%	0.467%
71	13.321	1941	1944	1947	rVV	72368	55027	2.81%	0.397%

LSC Area Percent Report

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Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.351	1947	1949	1953	rVB2	55648	46860	2.39%	0.338%
73	13.998	2054	2059	2062	rBV	920022	942266	48.11%	6.800%
74	14.021	2062	2063	2065	rVB	77855	42652	2.18%	0.308%
75	14.263	2101	2104	2105	rBV2	104409	102192	5.22%	0.738%
76	15.457	2303	2307	2314	rVB	789952	991528	50.63%	7.156%

Sum of corrected areas: 13856227

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060420\
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Operator : JU/CG
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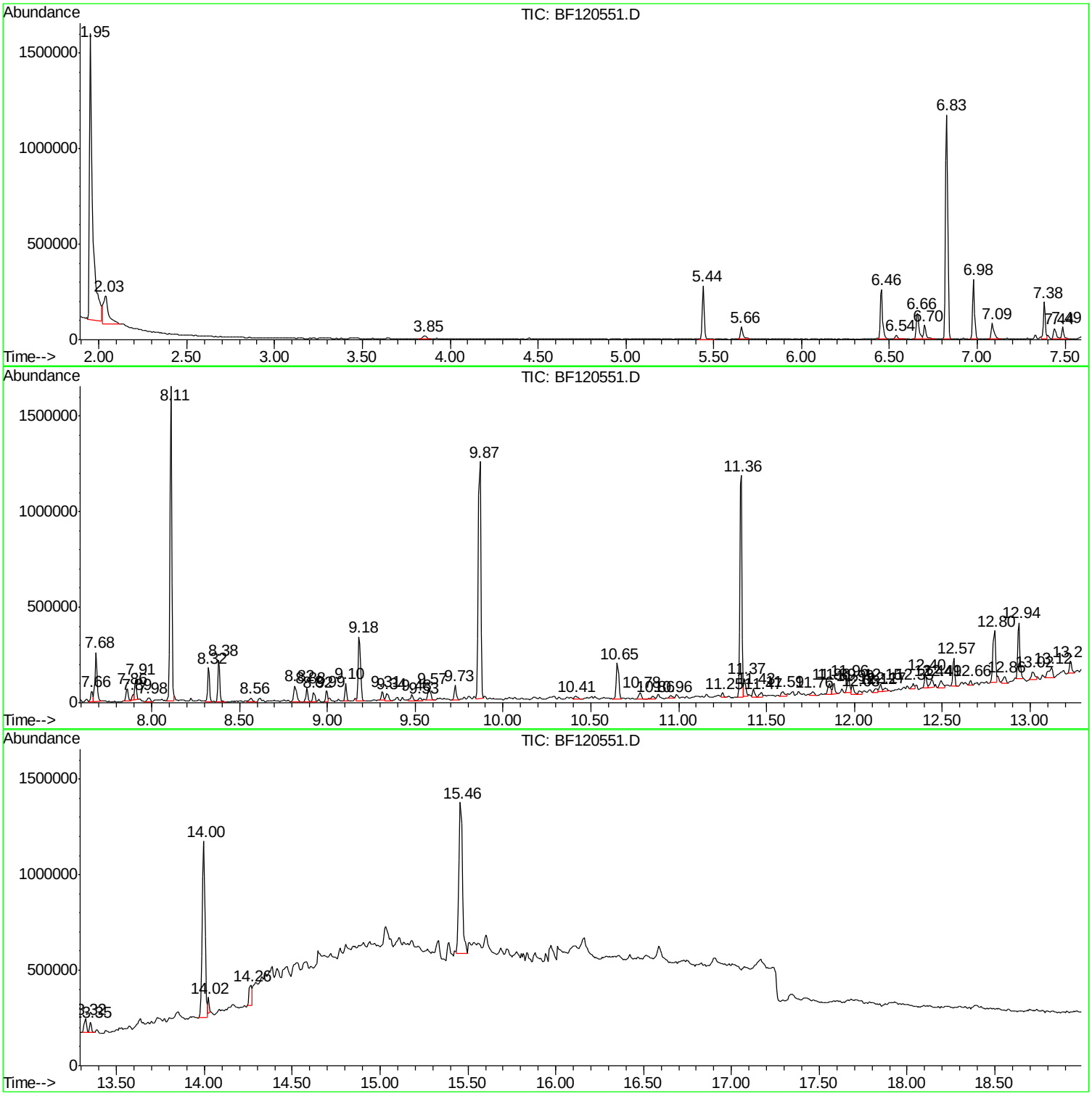
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060420\
Data File : BF120551.D
Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
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Instrument :
BNA_F
ClientSampleId :
CHRT27247

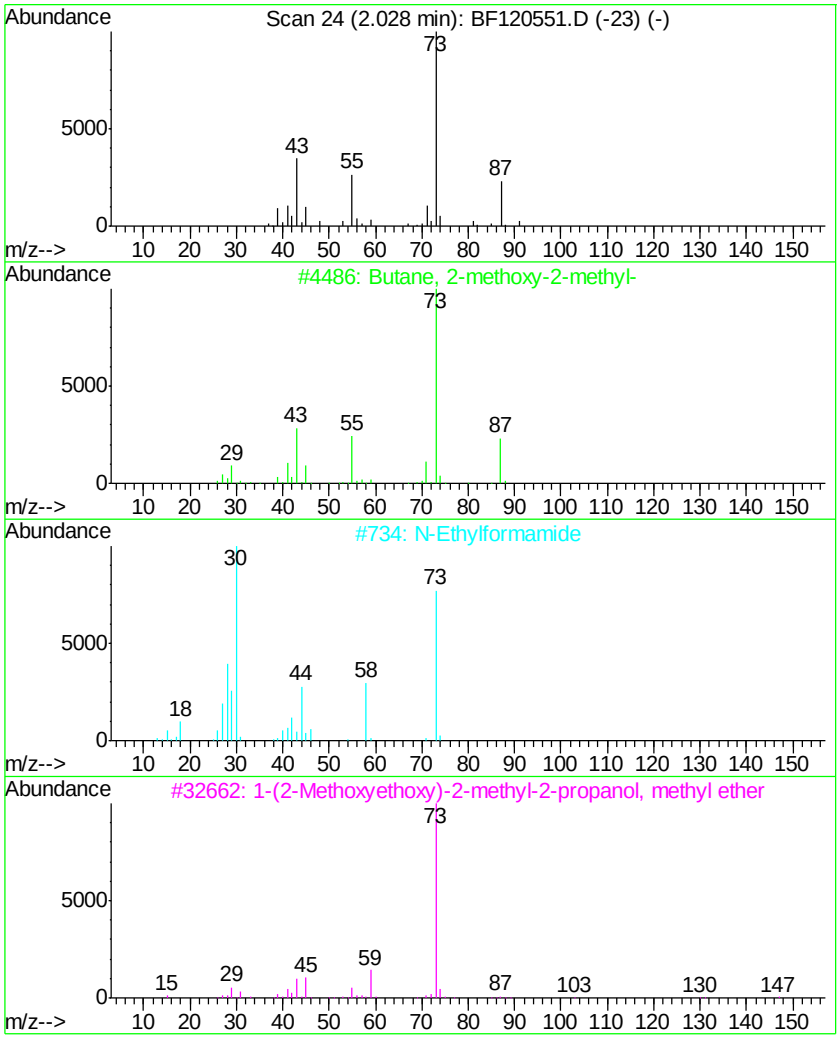
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

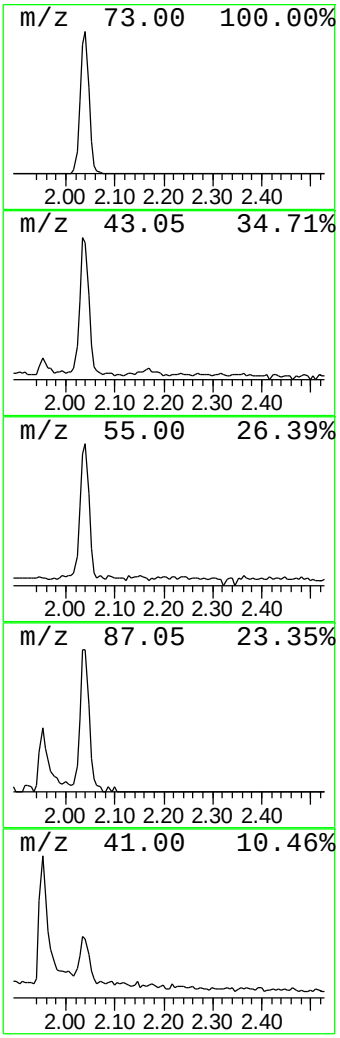
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.03	5.64 ng	267919	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060420\
Data File : BF120551.D
Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

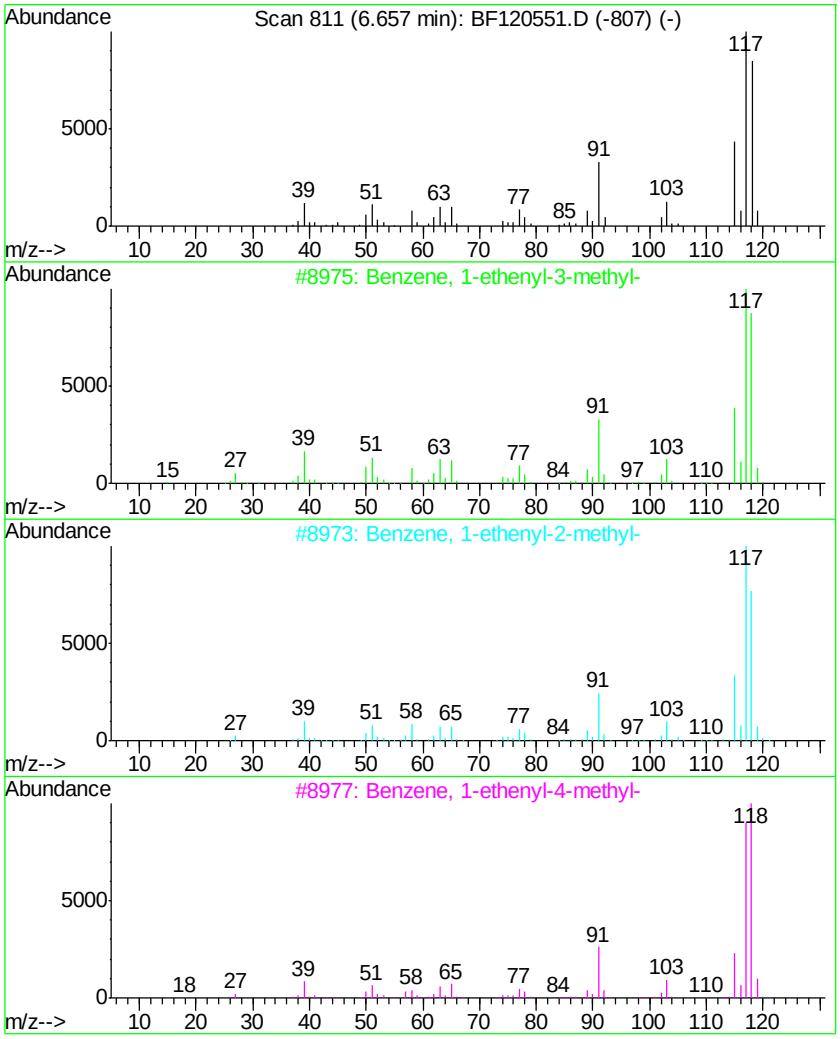
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

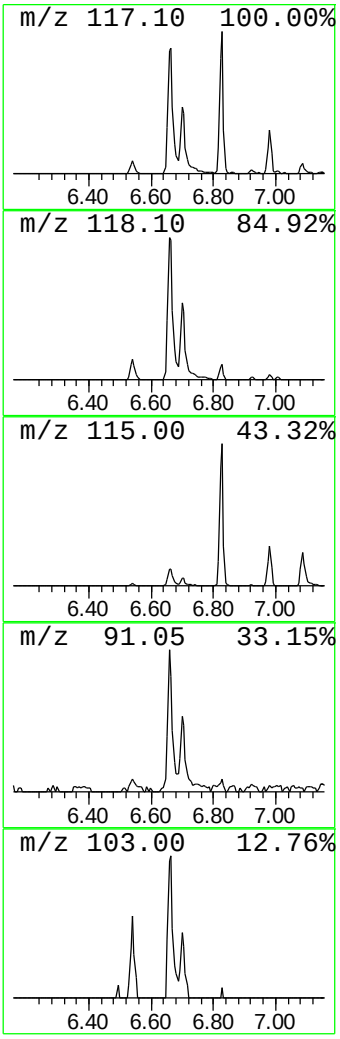
****

Peak Number 3 Benzene, 1-ethenyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	3.39 ng	161023	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	96
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	93
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060420\
Data File : BF120551.D
Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

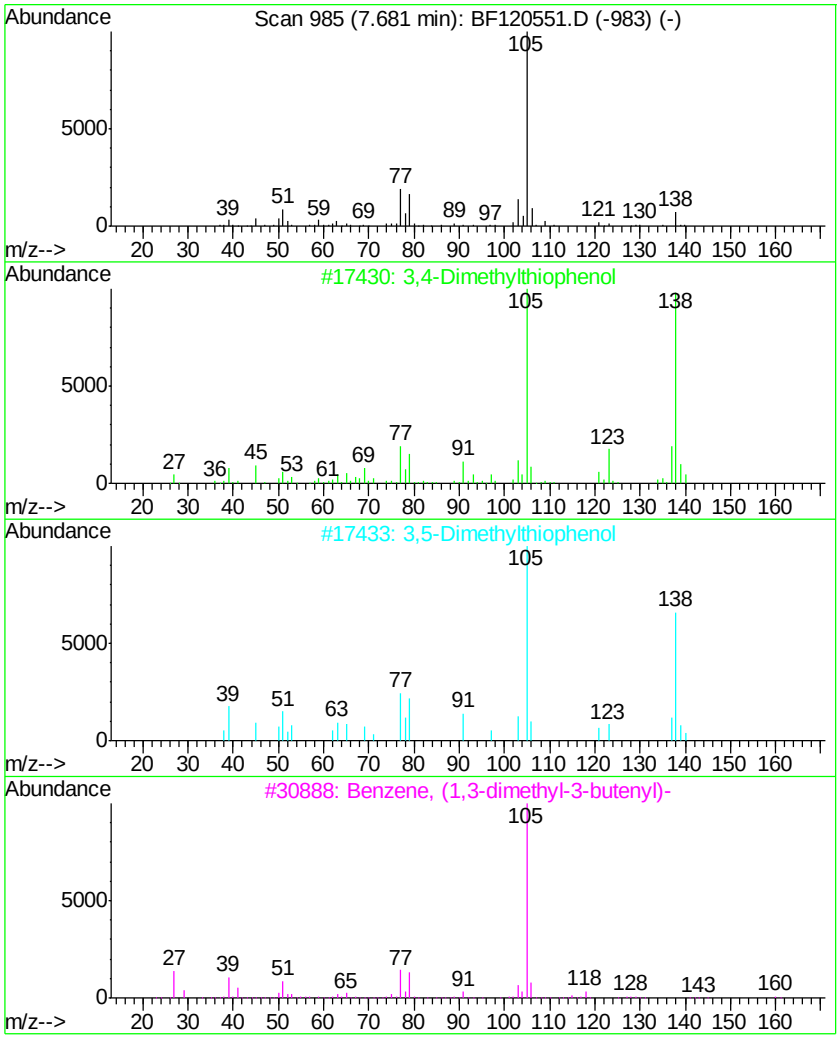
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

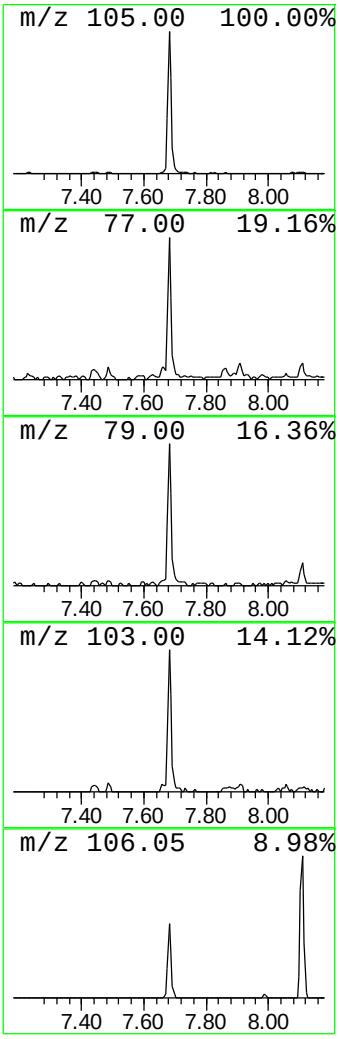
****

Peak Number 5 3,4-Dimethylthiophenol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	3.19 ng	212462	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylthiophenol	138	C8H10S	018800-53-8	78
2	3,5-Dimethylthiophenol	138	C8H10S	038360-81-5	72
3	Benzene, (1,3-dimethyl-3-butenyl)-	160	C12H16	056851-51-5	72
4	Phenol, o-[(.alpha.-methylbenzyl...	262	C14H14O3S	029634-38-6	59
5	Benzene, 1,1'-(1-methyl-1,2-etha...	196	C15H16	005814-85-7	59





Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

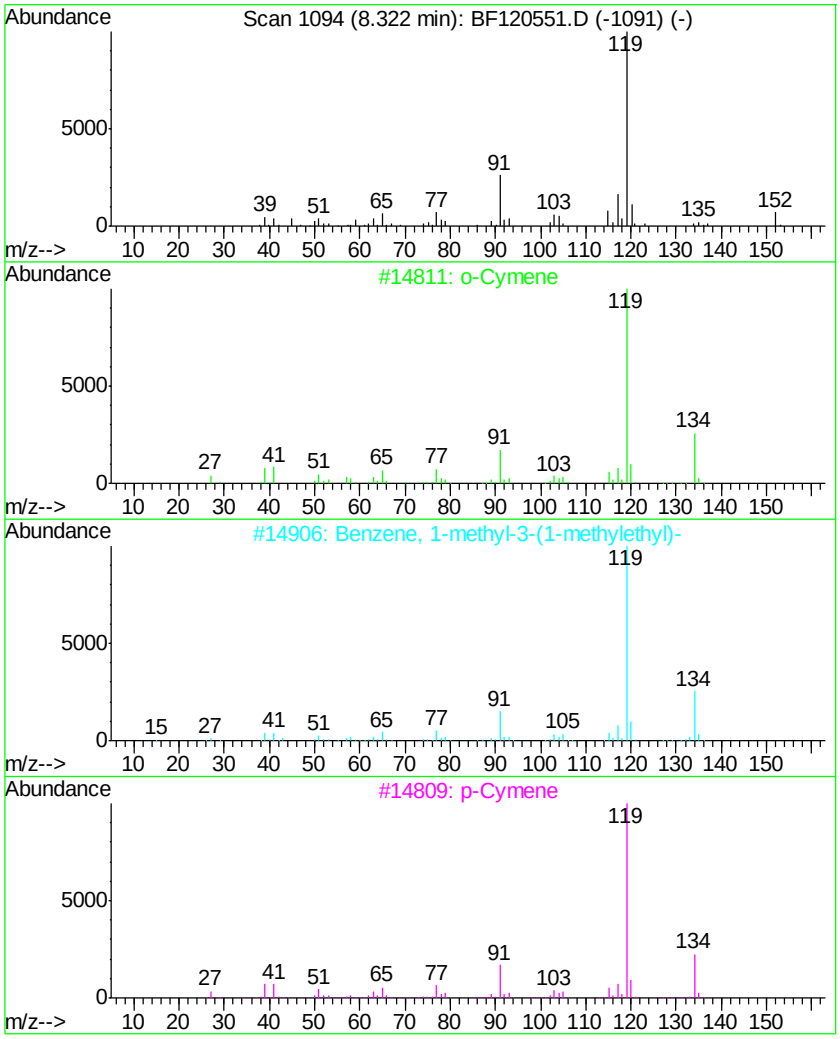
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

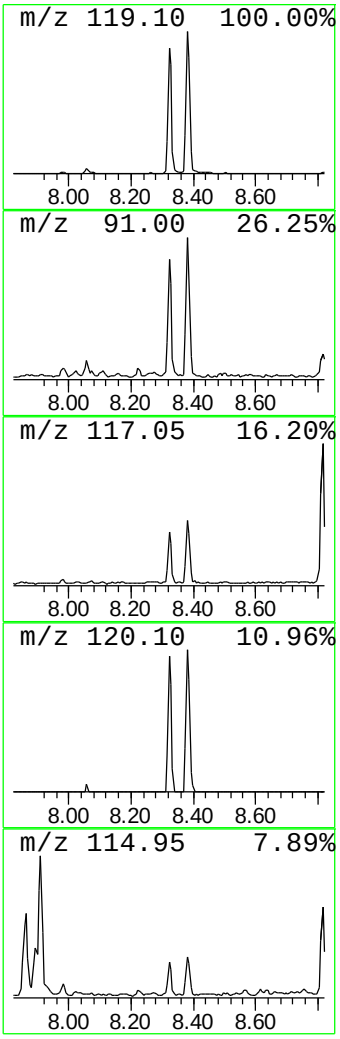
****

Peak Number 6 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	2.13 ng	141814	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	87
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	87
3	p-Cymene	134	C10H14	000099-87-6	87
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	80
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	80





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

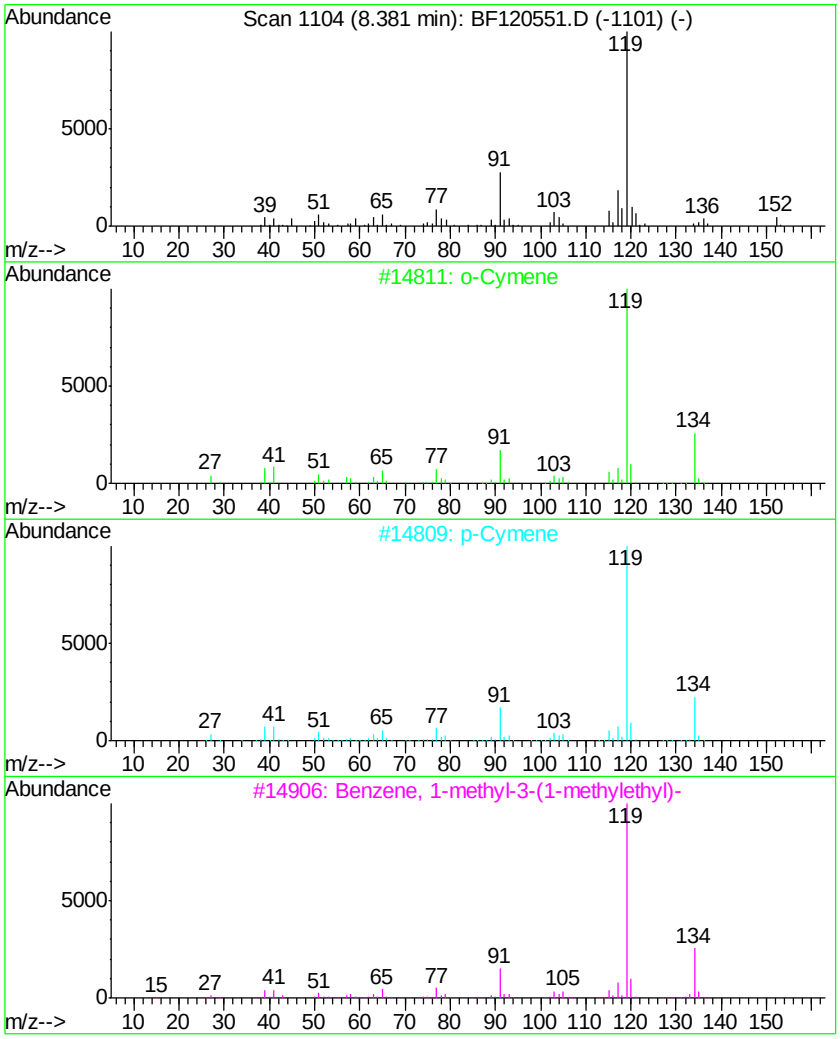
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

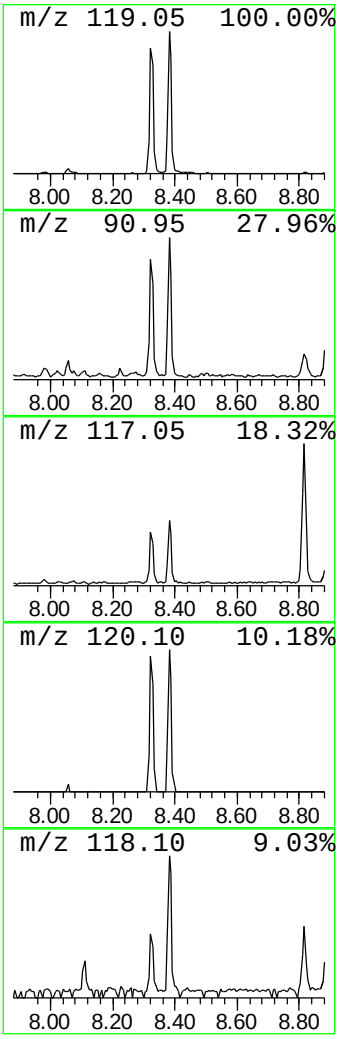
****

Peak Number 7 p-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	2.69 ng	179087	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	76
2	p-Cymene	134	C10H14	000099-87-6	76
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	76
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	68
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64





Library Search Compound Report

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Data File : BF120551.D
Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

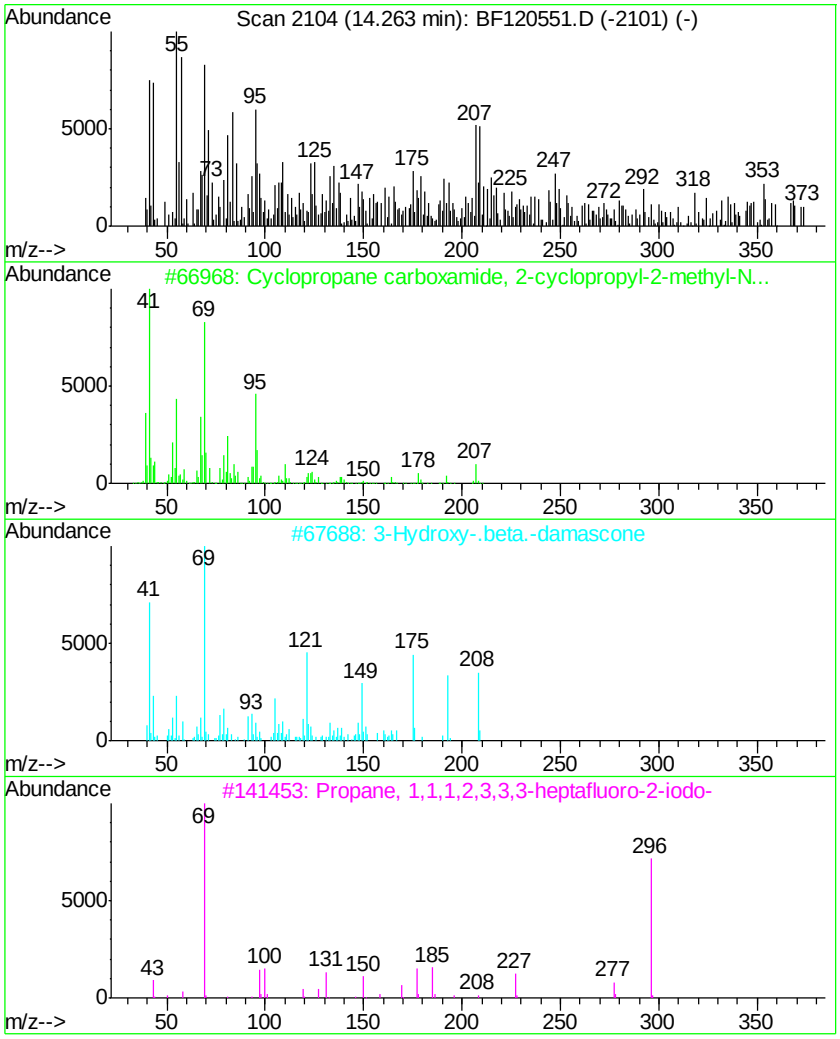
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

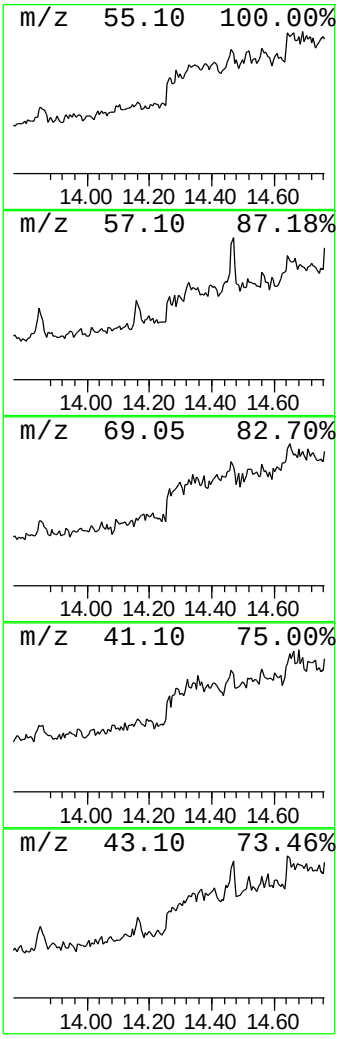
****

Peak Number 8 unknown14.26 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	2.17 ng	102192	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	49
2	3-Hydroxy-.beta.-damascone	208	C13H20O2	102488-09-5	30
3	Propane, 1,1,1,2,3,3,3-heptafluo...	296	C3F7I	000677-69-0	25
4	Benzoic acid, 4-(5-methyl-4-oxo-...	341	C19H19NO3S	296243-24-8	25
5	7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF060420\
Data File : BF120551.D
Acq On : 4 Jun 2020 23:29
Operator : JU/CG
Sample : L2858-01 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT27247

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF052820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	2.03	5.6	ng	267919	1	6.83	950502	20.0
Benzene, 1-etheny...	6.66	3.4	ng	161023	1	6.83	950502	20.0
3,4-Dimethylthiop...	7.68	3.2	ng	212462	2	8.11	1331390	20.0
o-Cymene	8.32	2.1	ng	141814	2	8.11	1331390	20.0
p-Cymene	8.38	2.7	ng	179087	2	8.11	1331390	20.0
unknown14.26	14.26	2.2	ng	102192	5	14.00	942266	20.0