LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098296.D
Acq On : 7 Sep 2017 2:15
Operator : SJ/JU
Sample : I5052-12 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G27A-1.5-3

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.657	92	97	103	rVB3	5756	10420	1.35%	0.135%
2	3.610	253	259	269	rVB	46451	75057	9.71%	0.971%
3	4.863	469	472	478	rBV2	24626	28624	3.70%	0.370%
4	5.298	542	546	555	rBV	380369	397266	51.37%	5.137%
5	6.334	719	722	734	rBV	474947	419815	54.29%	5.429%
6	6.463	740	744	748	rBV	508349	408696	52.85%	5.285%
7	6.698	780	784	787	rBV	688335	640646	82.84%	8.284%
8	6.851	806	810	817	rBV	371696	313983	40.60%	4.060%
9	7.257	876	879	884	rBV	255894	217224	28.09%	2.809%
10	7.298	884	886	889	rVB	12874	9936	1.28%	0.128%
11	7.981	998	1002	1005	rBV	945710	773337	100.00%	10.000%
12	8.404	1071	1074	1077	rBV	13487	12534	1.62%	0.162%
13	8.575	1101	1103	1106	rBV	15019	11107	1.44%	0.144%
14	8.692	1120	1123	1126	rBV	21635	16088	2.08%	0.208%
15	8.792	1137	1140	1144	rVB	16238	12145	1.57%	0.157%
16	9.051	1181	1184	1195	rBV	399801	370090	47.86%	4.786%
17	9.139	1195	1199	1203	rBV2	20405	20112	2.60%	0.260%
18	9.392	1239	1242	1244	rBV	12866	12233	1.58%	0.158%
19	9.451	1248	1252	1256	rVV2	46950	50102	6.48%	0.648%
20	9.592	1272	1276	1281	rBV	19303	19057	2.46%	0.246%
21	9.669	1286	1289	1293	rVB	20717	16400	2.12%	0.212%
22	9.733	1296	1300	1311	rVB	748400	677871	87.66%	8.766%
23	9.933	1331	1334	1338	rBV	10868	10650	1.38%	0.138%
24	10.139	1366	1369	1371	rBV3	12364	13790	1.78%	0.178%
25	10.169	1371	1374	1377	rVB	19954	18070	2.34%	0.234%
26	10.386	1405	1411	1415	rBV2	16616	18858	2.44%	0.244%
27	10.522	1430	1434	1441	rVB	153439	151705	19.62%	1.962%
28	10.651	1451	1456	1459	rBV4	37129	53369	6.90%	0.690%
29	11.086	1527	1530	1532	rBV2	28321	21385	2.77%	0.277%
30	11.116	1532	1535	1540	rVB2	20216	20736	2.68%	0.268%
31	11.216	1548	1552	1554	rBV	695817	598603	77.41%	7.741%
32	11.233	1554	1555	1558	rVV	50793	38963	5.04%	0.504%
33	11.292	1562	1565	1568	rVB	24309	23420	3.03%	0.303%
34	11.510	1600	1602	1606	rVB	23060	17300	2.24%	0.224%

LSC Area Percent Report

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Sample : I5052-12 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G27A-1.5-3

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.716	1635	1637	1639	rBV2	11042	9635	1.25%	0.125%
36	11.745	1639	1642	1645	rVV	20752	18014	2.33%	0.233%
37	11.780	1645	1648	1653	rVV3	9675	17697	2.29%	0.229%
38	11.827	1653	1656	1658	rVV2	19896	23707	3.07%	0.307%
39	11.851	1658	1660	1663	rVB2	12712	12016	1.55%	0.155%
40	11.916	1669	1671	1674	rBV	25238	22004	2.85%	0.285%
41	12.010	1685	1687	1690	rBV3	10666	12870	1.66%	0.166%
42	12.039	1690	1692	1695	rVB4	10790	10443	1.35%	0.135%
43	12.192	1715	1718	1725	rBV5	11779	22189	2.87%	0.287%
44	12.263	1727	1730	1733	rBV	22452	24675	3.19%	0.319%
45	12.304	1733	1737	1742	rVB3	30337	36695	4.75%	0.475%
46	12.351	1742	1745	1748	rBV2	17898	18518	2.39%	0.239%
47	12.421	1754	1757	1760	rBV	96184	83518	10.80%	1.080%
48	12.516	1771	1773	1776	rBV4	14302	18061	2.34%	0.234%
49	12.651	1791	1796	1798	rBV	107102	100014	12.93%	1.293%
50	12.680	1798	1801	1803	rVB3	26879	25962	3.36%	0.336%
51	12.792	1817	1820	1828	rVB	325073	324230	41.93%	4.193%
52	12.974	1846	1851	1855	rVB4	25810	41725	5.40%	0.540%
53	13.033	1858	1861	1866	rBV3	27399	31222	4.04%	0.404%
54	13.280	1901	1903	1907	rVB4	32780	32476	4.20%	0.420%
55	13.374	1917	1919	1922	rVB2	24700	19887	2.57%	0.257%
56	13.486	1936	1938	1943	rVB3	26320	32415	4.19%	0.419%
57	13.698	1972	1974	1978	rBV4	33526	34706	4.49%	0.449%
58	13.851	1995	2000	2003	rBV	643956	726206	93.91%	9.391%
59	14.621	2128	2131	2133	rBV	53025	62390	8.07%	0.807%
60	14.857	2169	2171	2174	rBV	62993	67498	8.73%	0.873%
61	15.262	2236	2240	2243	rBV	327604	404944	52.36%	5.236%

Sum of corrected areas: 7733309

LSC Report - Integrated Chromatogram

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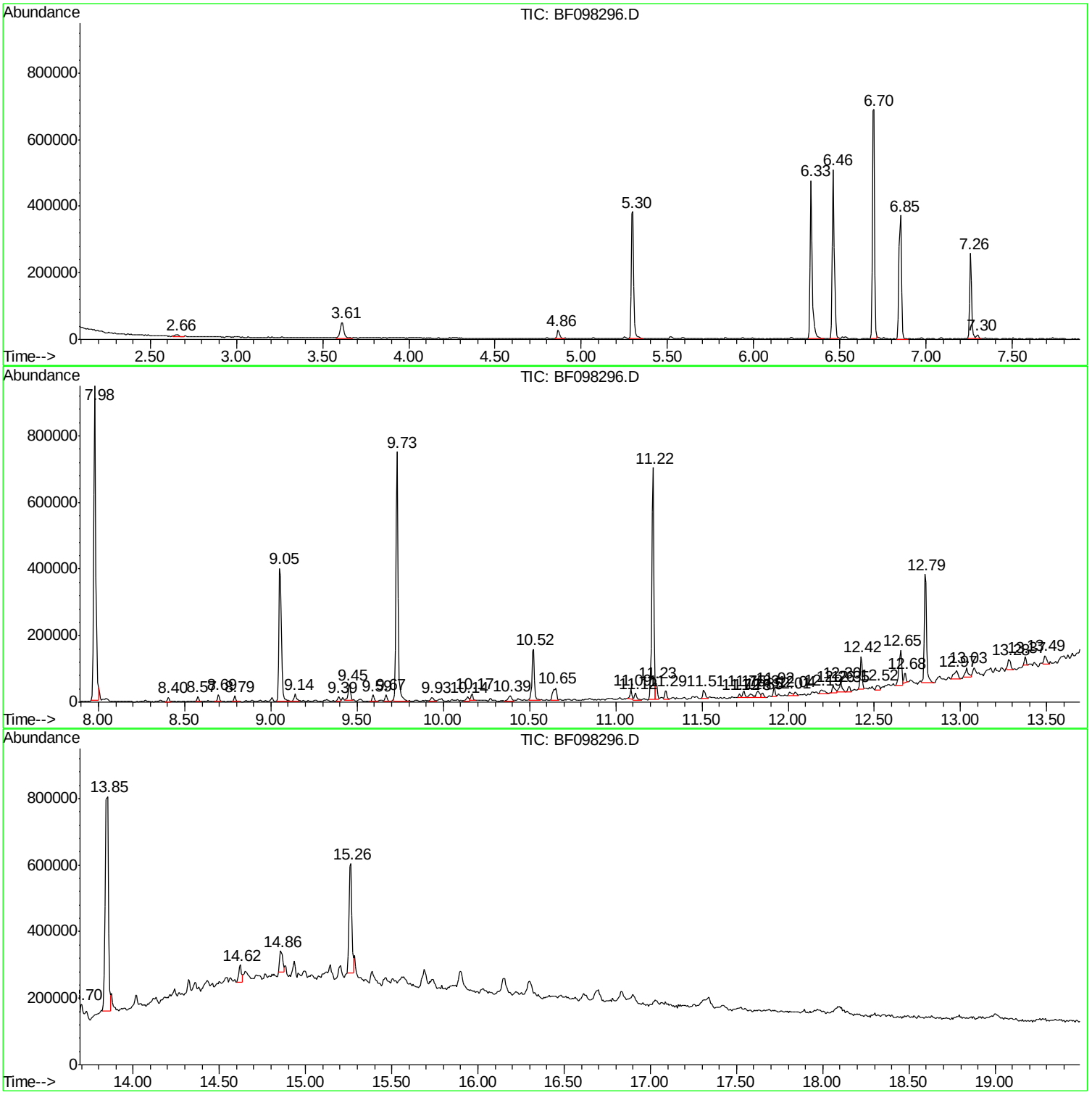
Operator : SJ/JU
Sample : I5052-12 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G27A-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098296.D
Acq On : 7 Sep 2017 2:15
Operator : SJ/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : G27A-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

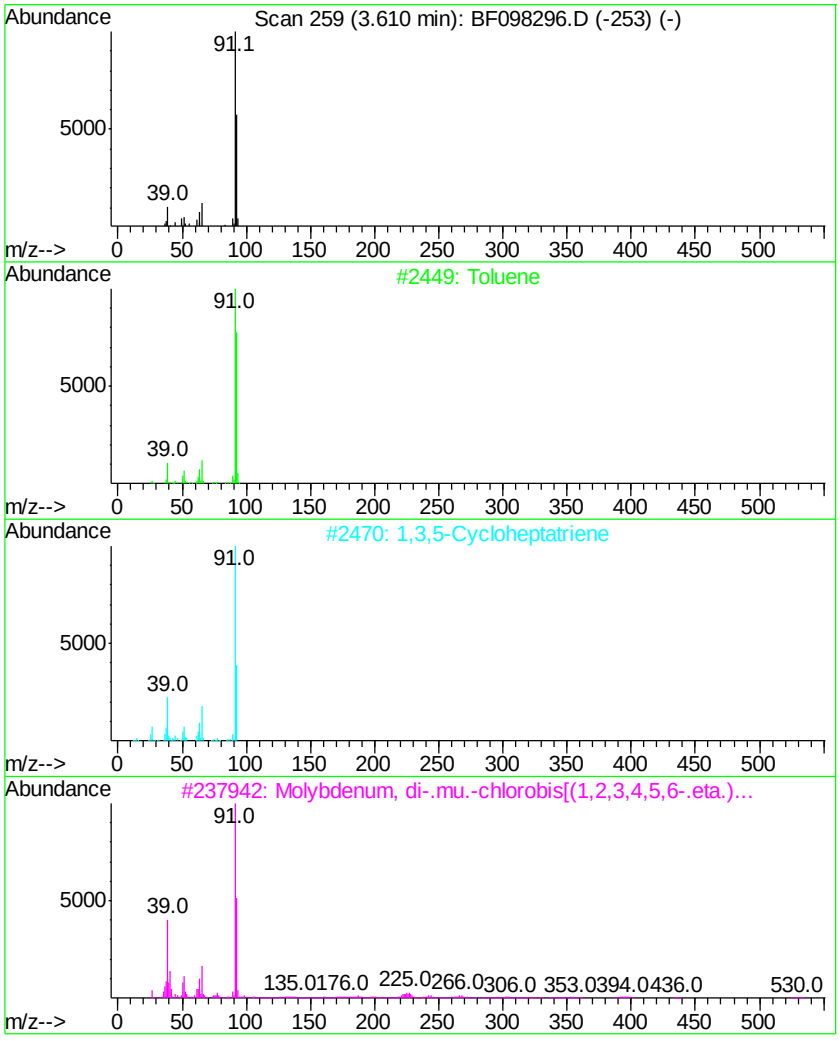
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

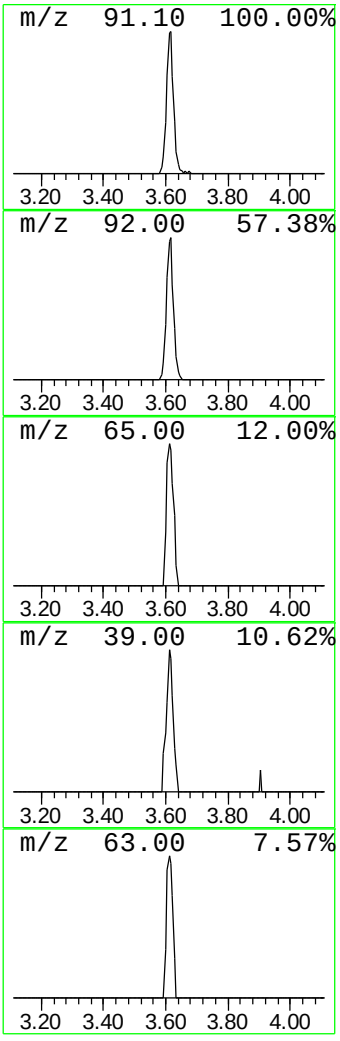
****

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	2.34 ng	75057	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	91
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	80
3	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	72
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	59
5	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	49





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Instrument : BNA_F
ClientSampleId : G27A-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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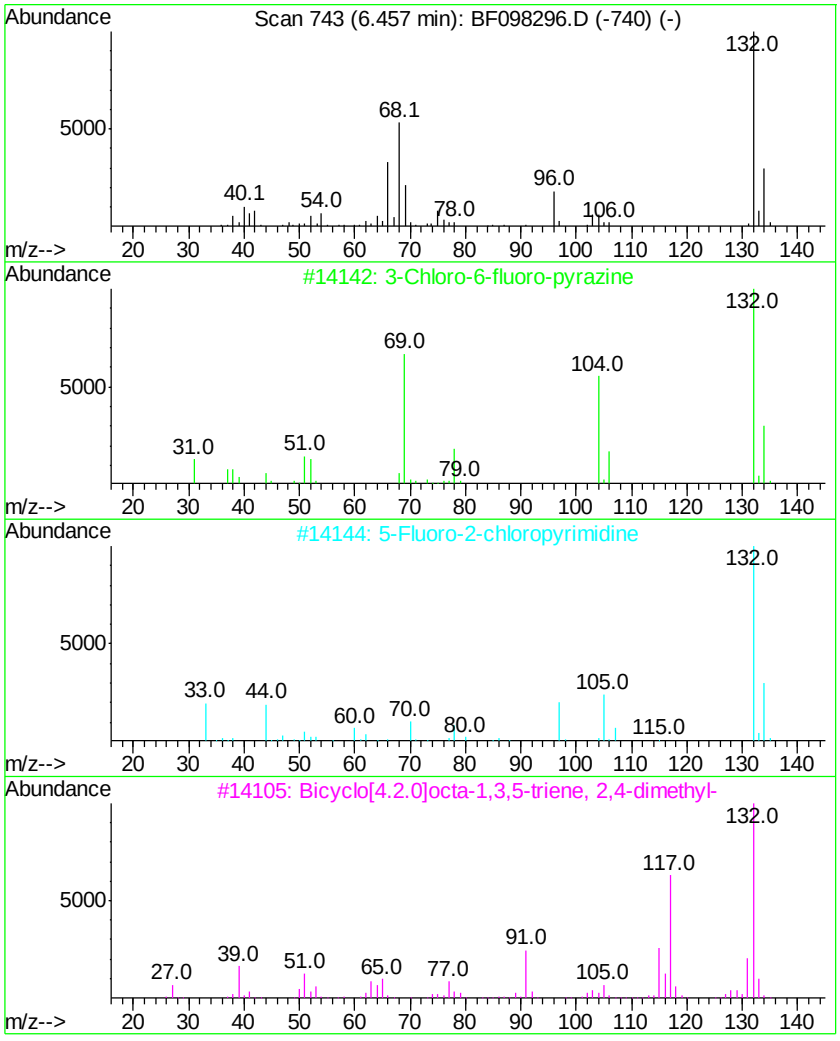
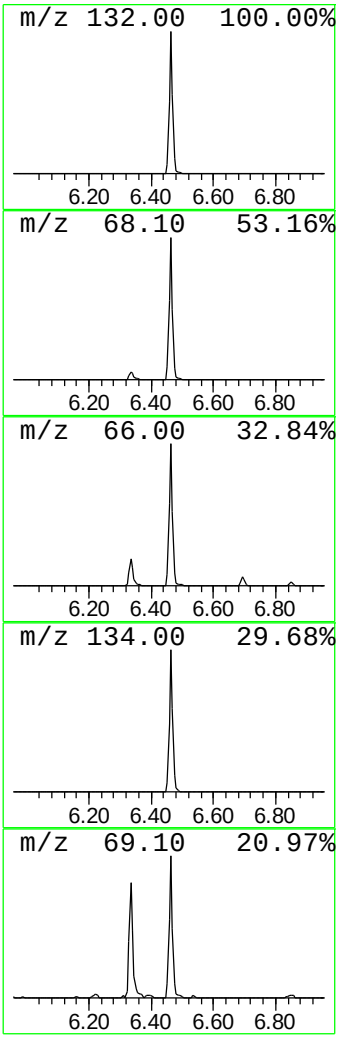
Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	12.76 ng	408696	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Xenon	132	Xe	007440-63-3	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090617\
Data File : BF098296.D
Acq On : 7 Sep 2017 2:15
Operator : SJ/JU
Sample : I5052-12 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G27A-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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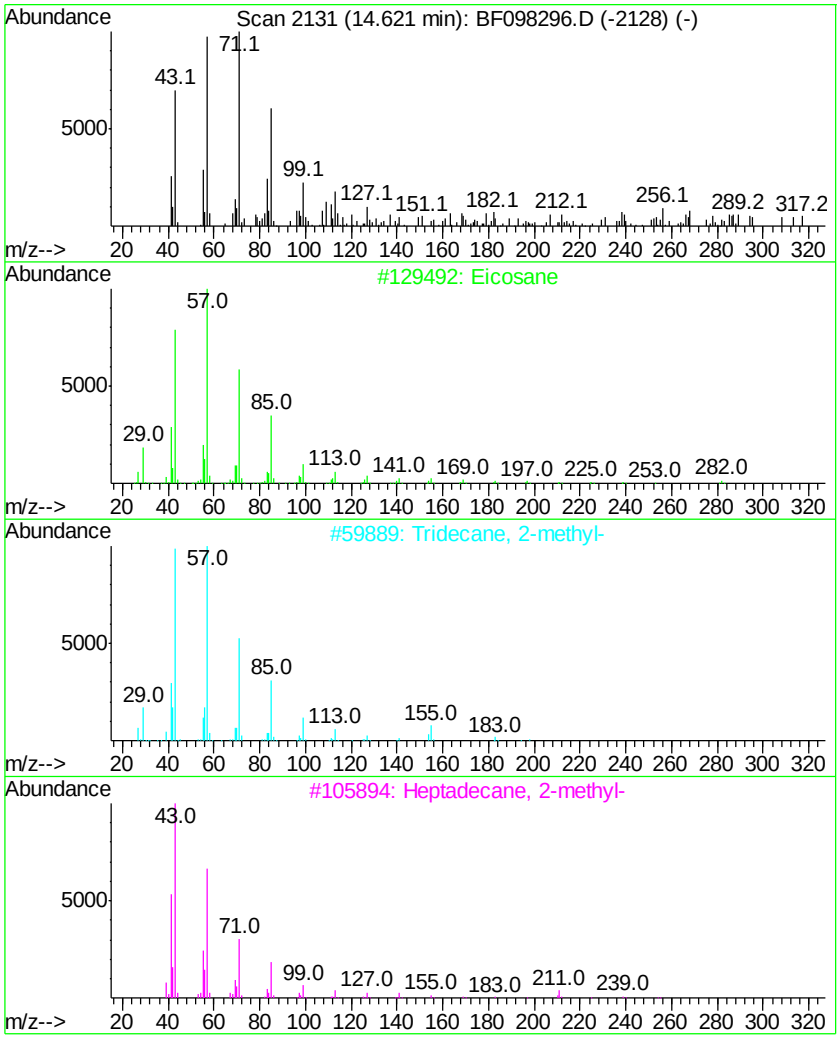
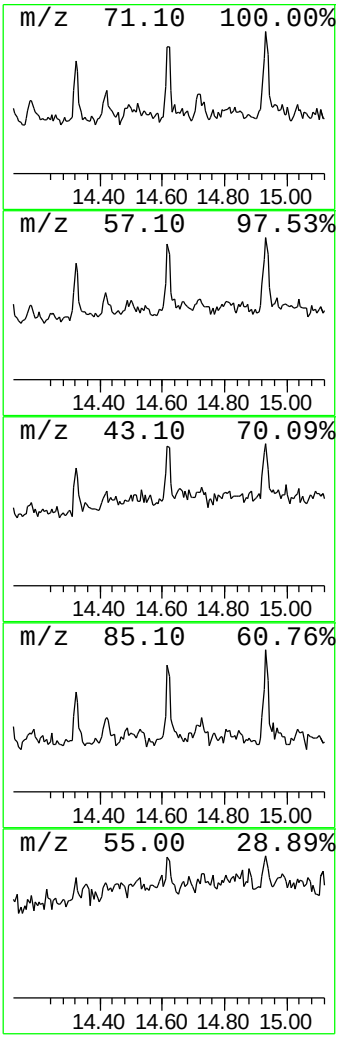
Peak Number 4 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.08 ng	62390	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	76
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	72
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	72
4	Nonadecane	268	C19H40	000629-92-5	68
5	Heneicosane	296	C21H44	000629-94-7	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3,5-Cycloheptat...	3.61	2.3	ng	75057	1	6.70	640646	20.0
unknown6.46	6.46	12.8	ng	408696	1	6.70	640646	20.0
Eicosane	14.62	3.1	ng	62390	6	15.26	404944	20.0