LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098931.D
Acq On : 29 Sep 2017 2:40
Operator : SJ/JU
Sample : I5487-04 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092717-B

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-BF092317.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	5.128	514	517	525	rBV	88775	85337	10.27%	0.910%
2	5.528	581	585	590	rBV	474800	421648	50.76%	4.496%
3	6.528	752	755	764	rVB	450033	393385	47.36%	4.195%
4	6.681	777	781	784	rBV	540478	423571	50.99%	4.517%
5	6.745	788	792	795	rBV3	11214	10354	1.25%	0.110%
6	6.916	817	821	824	rBV	904055	707094	85.12%	7.540%
7	7.069	843	847	851	rBV	399352	323865	38.99%	3.454%
8	7.469	912	915	919	rBV	257035	222101	26.74%	2.368%
9	8.198	1035	1039	1042	rBV	1063621	818380	98.52%	8.727%
10	8.781	1134	1138	1142	rVB	13527	13214	1.59%	0.141%
11	8.910	1156	1160	1164	rBV	33596	24643	2.97%	0.263%
12	9.010	1173	1177	1182	rVB	36841	32009	3.85%	0.341%
13	9.269	1216	1221	1231	rBV	469099	382069	46.00%	4.074%
14	9.345	1231	1234	1237	rBV	20679	17668	2.13%	0.188%
15	9.539	1263	1267	1271	rBV2	19011	24684	2.97%	0.263%
16	9.610	1275	1279	1281	rBV	33857	34855	4.20%	0.372%
17	9.663	1285	1288	1296	rVB	72416	74387	8.96%	0.793%
18	9.728	1296	1299	1301	rBV2	18729	15266	1.84%	0.163%
19	9.816	1311	1314	1317	rBV	36516	34568	4.16%	0.369%
20	9.875	1317	1324	1329	rVV3	26143	37621	4.53%	0.401%
21	9.951	1329	1337	1341	rVV	762051	731451	88.06%	7.800%
22	9.986	1341	1343	1351	rVB	41522	41600	5.01%	0.444%
23	10.157	1369	1372	1375	rVB2	22835	22171	2.67%	0.236%
24	10.192	1375	1378	1382	rBV3	19036	16340	1.97%	0.174%
25	10.269	1386	1391	1394	rBV4	10591	12411	1.49%	0.132%
26	10.375	1401	1409	1412	rBV2	26738	33047	3.98%	0.352%
27	10.498	1427	1430	1436	rVB	40100	37105	4.47%	0.396%
28	10.592	1443	1446	1448	rBV2	12030	11766	1.42%	0.125%
29	10.651	1451	1456	1459	rBV6	5787	11070	1.33%	0.118%
30	10.739	1468	1471	1475	rVB	188310	156958	18.90%	1.674%
31	10.845	1486	1489	1490	rBV	27039	22291	2.68%	0.238%
32	10.863	1490	1492	1495	rVB3	26097	22137	2.66%	0.236%
33	11.045	1519	1523	1526	rBV3	17039	23453	2.82%	0.250%
34	11.074	1526	1528	1532	rVB3	14330	12228	1.47%	0.130%

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092717-B

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.292	1562	1565	1567	rBV2	17421	12932	1.56%	0.138%
36	11.322	1567	1570	1577	rVB3	18263	28359	3.41%	0.302%
37	11.386	1577	1581	1586	rBV2	17811	22995	2.77%	0.245%
38	11.439	1586	1590	1593	rBV	758957	673872	81.12%	7.186%
39	11.463	1593	1594	1598	rVV	196143	121407	14.62%	1.295%
40	11.516	1600	1603	1606	rVB	69005	50008	6.02%	0.533%
41	11.604	1614	1618	1622	rVB6	6212	11237	1.35%	0.120%
42	11.669	1626	1629	1632	rVV	23263	24170	2.91%	0.258%
43	11.722	1635	1638	1643	rVV3	13341	19166	2.31%	0.204%
44	11.769	1644	1646	1652	rVB2	13077	13224	1.59%	0.141%
45	11.816	1652	1654	1658	rVB	14562	12920	1.56%	0.138%
46	11.857	1658	1661	1664	rBV3	10866	13610	1.64%	0.145%
47	11.939	1673	1675	1678	rBV	38714	39787	4.79%	0.424%
48	11.969	1678	1680	1685	rVB	53109	43275	5.21%	0.461%
49	12.016	1685	1688	1691	rBV	27642	21867	2.63%	0.233%
50	12.057	1691	1695	1697	rBV	67927	83272	10.02%	0.888%
51	12.127	1705	1707	1711	rBV4	12696	13192	1.59%	0.141%
52	12.233	1722	1725	1728	rBV	37987	30884	3.72%	0.329%
53	12.257	1728	1729	1736	rVB5	10712	15585	1.88%	0.166%
54	12.416	1754	1756	1758	rBV2	16609	12225	1.47%	0.130%
55	12.439	1758	1760	1762	rVB2	16664	11985	1.44%	0.128%
56	12.492	1765	1769	1771	rBV	44228	47794	5.75%	0.510%
57	12.527	1771	1775	1777	rVV4	28207	39136	4.71%	0.417%
58	12.574	1781	1783	1789	rBV6	24616	44333	5.34%	0.473%
59	12.651	1793	1796	1800	rBV	240323	212079	25.53%	2.262%
60	12.751	1810	1813	1815	rVB2	13749	12994	1.56%	0.139%
61	12.804	1820	1822	1825	rVV3	17976	18527	2.23%	0.198%
62	12.886	1829	1836	1842	rVV	259386	302793	36.45%	3.229%
63	12.939	1842	1845	1848	rVB4	19588	23686	2.85%	0.253%
64	12.998	1853	1855	1856	rBV2	15569	12703	1.53%	0.135%
65	13.021	1856	1859	1862	rVV	388742	316204	38.07%	3.372%
66	13.098	1869	1872	1875	rBV3	26778	37408	4.50%	0.399%
67	13.186	1884	1887	1888	rBV3	26916	27396	3.30%	0.292%
68	13.210	1888	1891	1894	rVB	60433	59777	7.20%	0.637%
69	13.245	1894	1897	1899	rBV4	17753	21732	2.62%	0.232%
70	13.274	1900	1902	1905	rVV	41509	35098	4.23%	0.374%
71	13.316	1906	1909	1912	rVV	47976	41859	5.04%	0.446%

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Instrument : BNA_F
ClientSampleId : CL-02-092717-B

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.410	1922	1925	1927	rBV	28191	24778	2.98%	0.264%
73	13.439	1927	1930	1932	rBV	35667	30120	3.63%	0.321%
74	14.051	2031	2034	2035	rBV	42645	42567	5.12%	0.454%
75	14.080	2035	2039	2042	rVV	811050	830673	100.00%	8.858%
76	14.104	2042	2043	2049	rVB	117863	101639	12.24%	1.084%
77	15.580	2289	2294	2302	rVB	410241	567620	68.33%	6.053%

Sum of corrected areas: 9377635

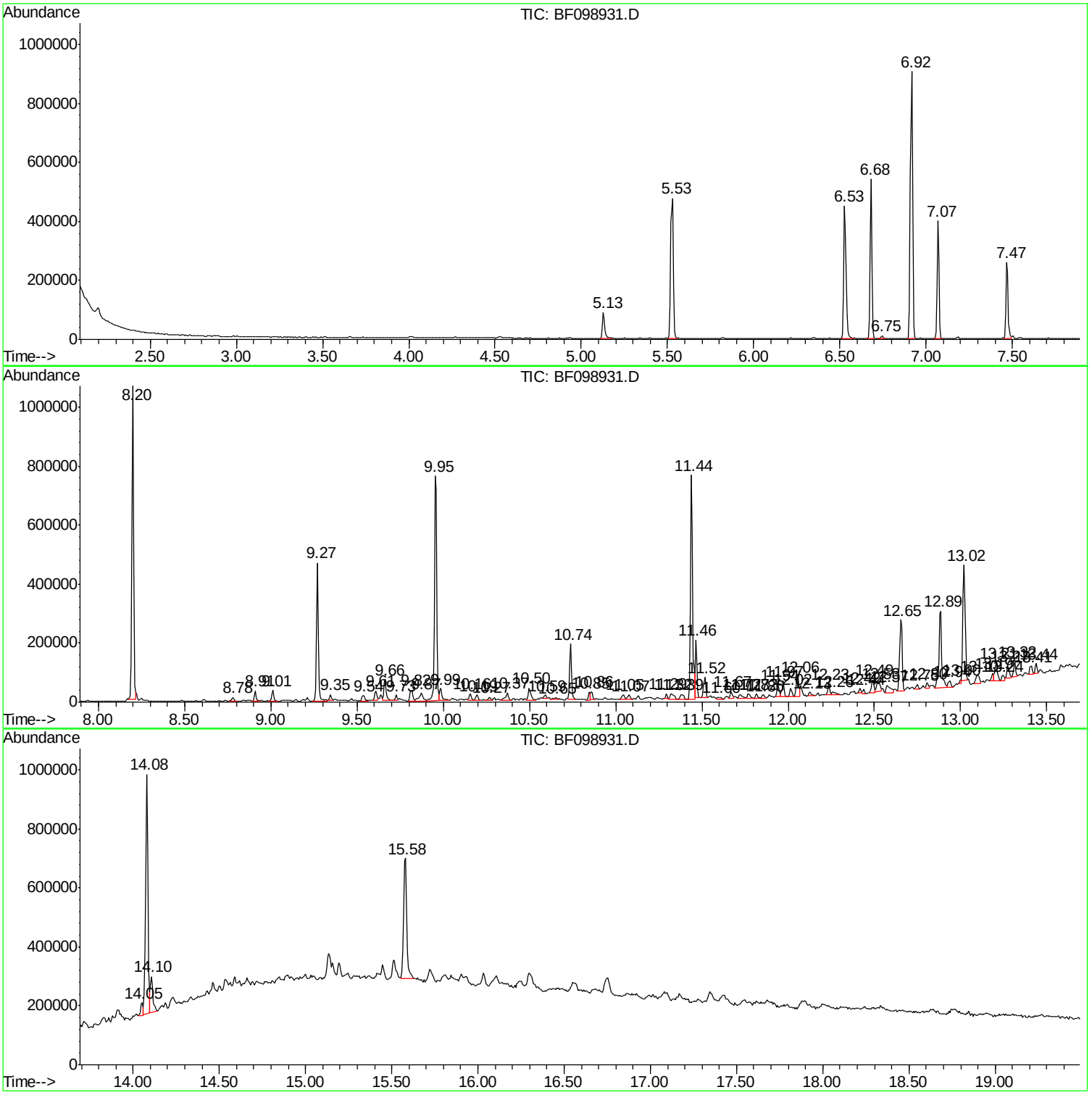
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098931.D
Acq On : 29 Sep 2017 2:40
Operator : SJ/JU
Sample : I5487-04 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-092717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098931.D
Acq On : 29 Sep 2017 2:40
Operator : SJ/JU
Sample : I5487-04 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-092717-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

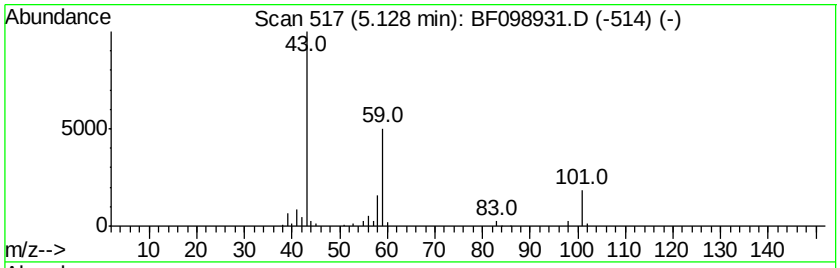
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

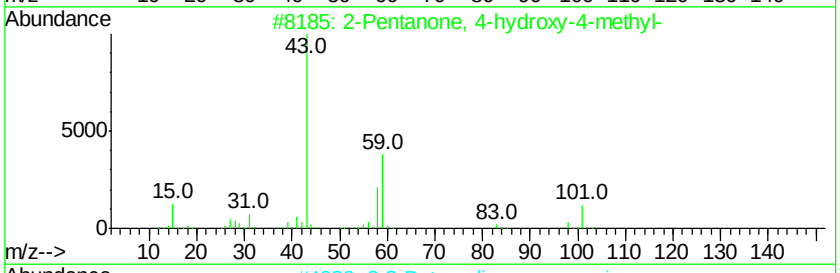
****

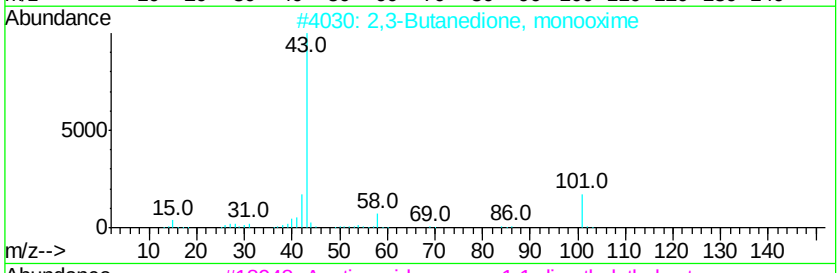
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

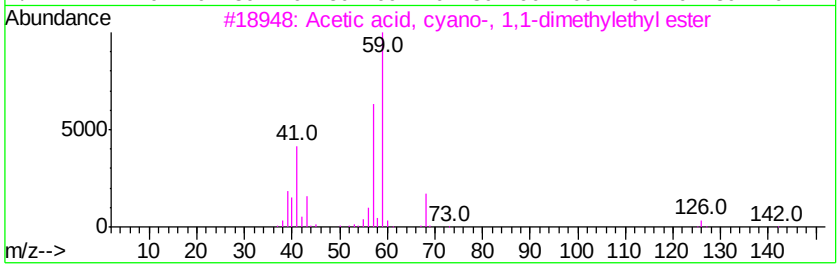
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	2.41 ng	85337	1,4-Dichlorobenzene-d4	6.92

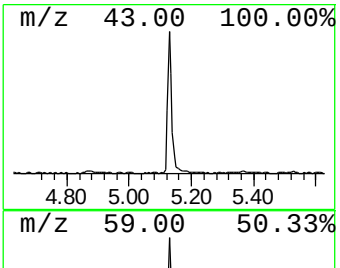
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9

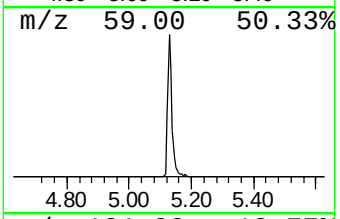


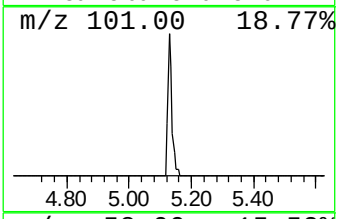


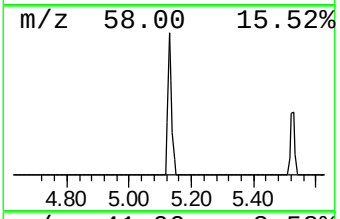


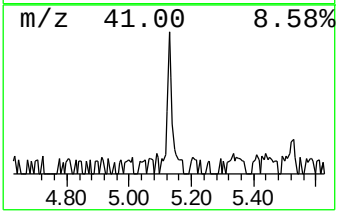












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

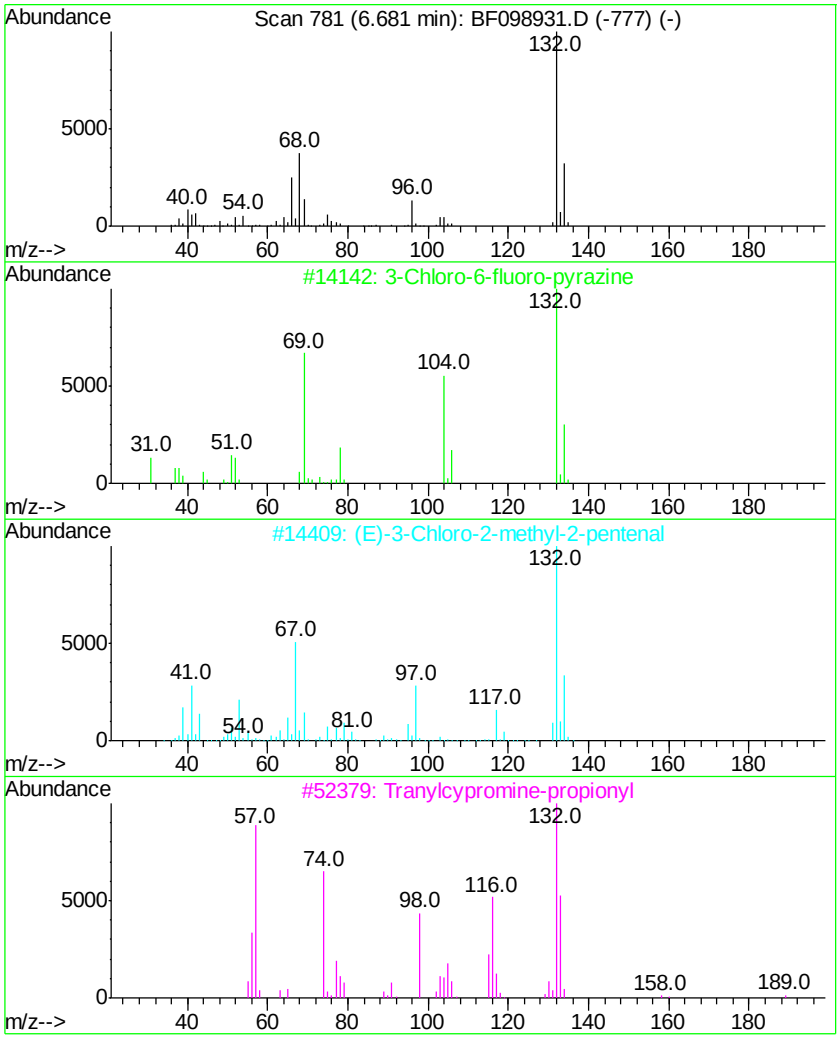
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

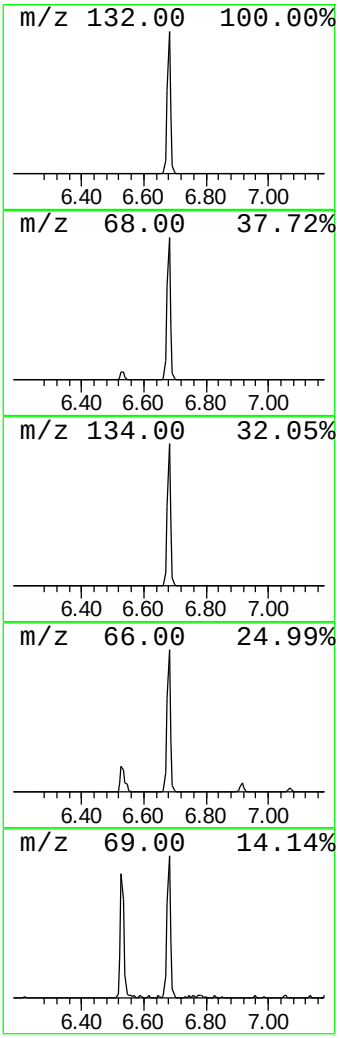
****

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	11.98 ng	423571	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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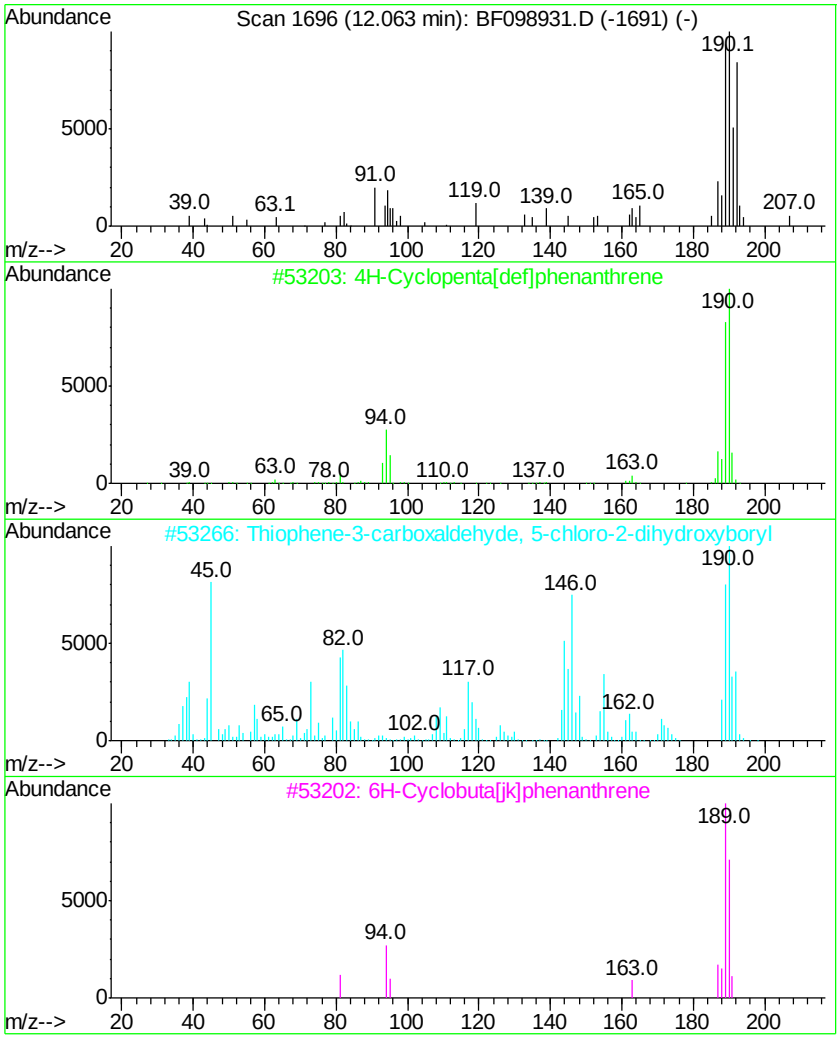
TIC Integration Parameters: LSCINT.P

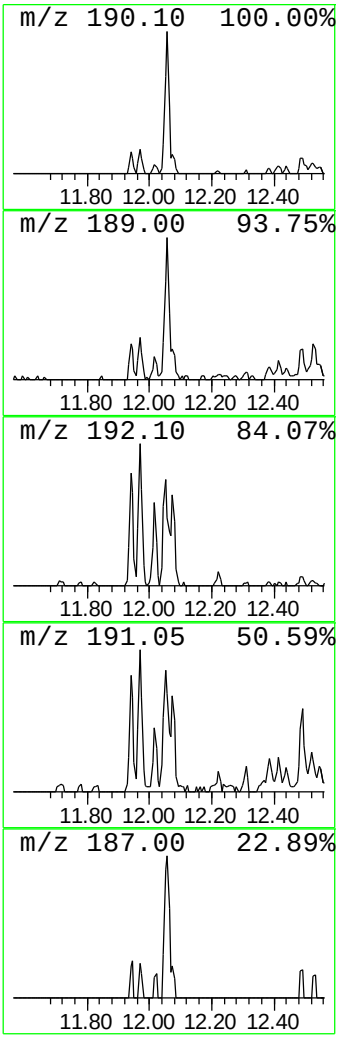
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	2.47 ng	83272	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
4	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
5	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	49





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	2.4	ng	85337	1	6.92	707094	20.0
unknown6.68	6.68	12.0	ng	423571	1	6.92	707094	20.0
4H-Cyclopenta[def...	12.06	2.5	ng	83272	4	11.44	673872	20.0