LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

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-BF090518.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	2.466	17	22	29	rVB	195044	285789	10.15%	0.843%
2	4.913	435	438	448	rVB	34657	37323	1.33%	0.110%
3	5.331	505	509	513	rVB	1028231	897599	31.89%	2.649%
4	6.354	679	683	686	rBV	1300866	997533	35.44%	2.944%
5	6.495	703	707	711	rBV	1213247	987196	35.07%	2.914%
6	6.736	744	748	751	rVB	1965475	1736998	61.71%	5.127%
7	6.889	770	774	777	rBV	995631	767529	27.27%	2.265%
8	7.289	837	842	845	rBV	643857	566548	20.13%	1.672%
9	8.013	961	965	968	rBV	2491189	2241456	79.64%	6.615%
10	8.725	1083	1086	1089	rVB2	42347	34962	1.24%	0.103%
11	9.089	1144	1148	1151	rBV	1562634	1108749	39.39%	3.272%
12	9.483	1211	1215	1218	rBV	325482	249780	8.87%	0.737%
13	9.625	1235	1239	1241	rBV	69765	57883	2.06%	0.171%
14	9.766	1259	1263	1266	rBV	2562121	2152957	76.49%	6.354%
15	9.795	1266	1268	1271	rVB	162453	121079	4.30%	0.357%
16	9.966	1294	1297	1301	rVB	74386	57908	2.06%	0.171%
17	10.183	1328	1334	1337	rBV5	19169	31556	1.12%	0.093%
18	10.283	1347	1351	1353	rBV	192107	159507	5.67%	0.471%
19	10.307	1353	1355	1358	rVB	114405	84599	3.01%	0.250%
20	10.389	1368	1369	1372	rVB2	43025	31513	1.12%	0.093%
21	10.542	1392	1395	1399	rBV	565667	446230	15.85%	1.317%
22	10.583	1399	1402	1406	rVB	76912	73472	2.61%	0.217%
23	10.683	1414	1419	1420	rBV4	25385	32159	1.14%	0.095%
24	11.042	1478	1480	1485	rVB	46418	38982	1.38%	0.115%
25	11.101	1487	1490	1493	rVV4	28704	47637	1.69%	0.141%
26	11.136	1493	1496	1498	rVB2	64145	57715	2.05%	0.170%
27	11.242	1510	1514	1516	rBV	2115808	1911915	67.93%	5.643%
28	11.266	1516	1518	1521	rVV	975023	762712	27.10%	2.251%
29	11.313	1523	1526	1529	rVV	301923	243692	8.66%	0.719%
30	11.348	1529	1532	1535	rVB3	39278	45869	1.63%	0.135%
31	11.448	1546	1549	1550	rBV	89787	71099	2.53%	0.210%
32	11.466	1550	1552	1555	rVB	107850	83371	2.96%	0.246%
33	11.742	1595	1599	1601	rBV	119319	115505	4.10%	0.341%
34	11.766	1601	1603	1608	rVV	165506	178710	6.35%	0.527%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

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-BF090518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.813	1608	1611	1614	rVB	122266	104740	3.72%	0.309%
36	11.848	1614	1617	1623	rBV	227995	312201	11.09%	0.921%
37	12.036	1646	1649	1650	rBV	101629	97637	3.47%	0.288%
38	12.183	1672	1674	1677	rBV2	33040	31365	1.11%	0.093%
39	12.236	1681	1683	1685	rVB3	37940	31754	1.13%	0.094%
40	12.289	1689	1692	1695	rVV	63636	69755	2.48%	0.206%
41	12.324	1695	1698	1700	rVV3	51870	56803	2.02%	0.168%
42	12.371	1703	1706	1711	rVB3	87029	125368	4.45%	0.370%
43	12.448	1715	1719	1722	rVB	1778334	1508461	53.59%	4.452%
44	12.518	1728	1731	1735	rVB	3066930	2814644	100.00%	8.307%
45	12.595	1742	1744	1749	rVB2	56462	52676	1.87%	0.155%
46	12.671	1752	1757	1760	rBV	1611409	1579975	56.13%	4.663%
47	12.718	1763	1765	1770	rVB3	124512	104872	3.73%	0.310%
48	12.766	1770	1773	1775	rBV	51667	51107	1.82%	0.151%
49	12.795	1775	1778	1779	rBV	84487	71213	2.53%	0.210%
50	12.818	1779	1782	1789	rVB	1050545	930883	33.07%	2.747%
51	12.889	1790	1794	1797	rBV3	98743	163230	5.80%	0.482%
52	12.977	1806	1809	1811	rBV3	82897	93719	3.33%	0.277%
53	13.001	1811	1813	1816	rVB	226872	183665	6.53%	0.542%
54	13.065	1822	1824	1827	rBV	166765	140808	5.00%	0.416%
55	13.101	1827	1830	1833	rBV2	149444	153341	5.45%	0.453%
56	13.195	1844	1846	1849	rBV	92147	76887	2.73%	0.227%
57	13.224	1849	1851	1857	rBV2	83327	108267	3.85%	0.320%
58	13.301	1861	1864	1867	rVB	761237	598346	21.26%	1.766%
59	13.501	1896	1898	1904	rVB	96020	100837	3.58%	0.298%
60	13.613	1914	1917	1920	rBV2	124067	157896	5.61%	0.466%
61	13.642	1920	1922	1924	rVV	131056	114004	4.05%	0.336%
62	13.665	1924	1926	1927	rVV	100681	76395	2.71%	0.225%
63	13.707	1931	1933	1935	rVV	101083	73228	2.60%	0.216%
64	13.865	1955	1960	1962	rBV2	2496770	2770408	98.43%	8.177%
65	13.889	1962	1964	1967	rVB	704495	534735	19.00%	1.578%
66	13.971	1975	1978	1981	rBV	112026	106995	3.80%	0.316%
67	14.083	1994	1997	1999	rBV2	93520	98268	3.49%	0.290%
68	14.871	2127	2131	2134	rBV	526216	781053	27.75%	2.305%
69	14.971	2146	2148	2155	rVB	237189	251134	8.92%	0.741%
70	15.154	2176	2179	2184	rVB	322900	356661	12.67%	1.053%
71	15.207	2185	2188	2193	rVB	426778	472135	16.77%	1.393%

LSC Area Percent Report

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Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

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-BF090518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	15.271	2194	2199	2202	rBV	1019515	1190529	42.30%	3.514%
73	16.612	2423	2427	2434	rVB2	183883	358488	12.74%	1.058%
74	17.018	2493	2496	2508	rVB	145145	260010	9.24%	0.767%

Sum of corrected areas: 33882025

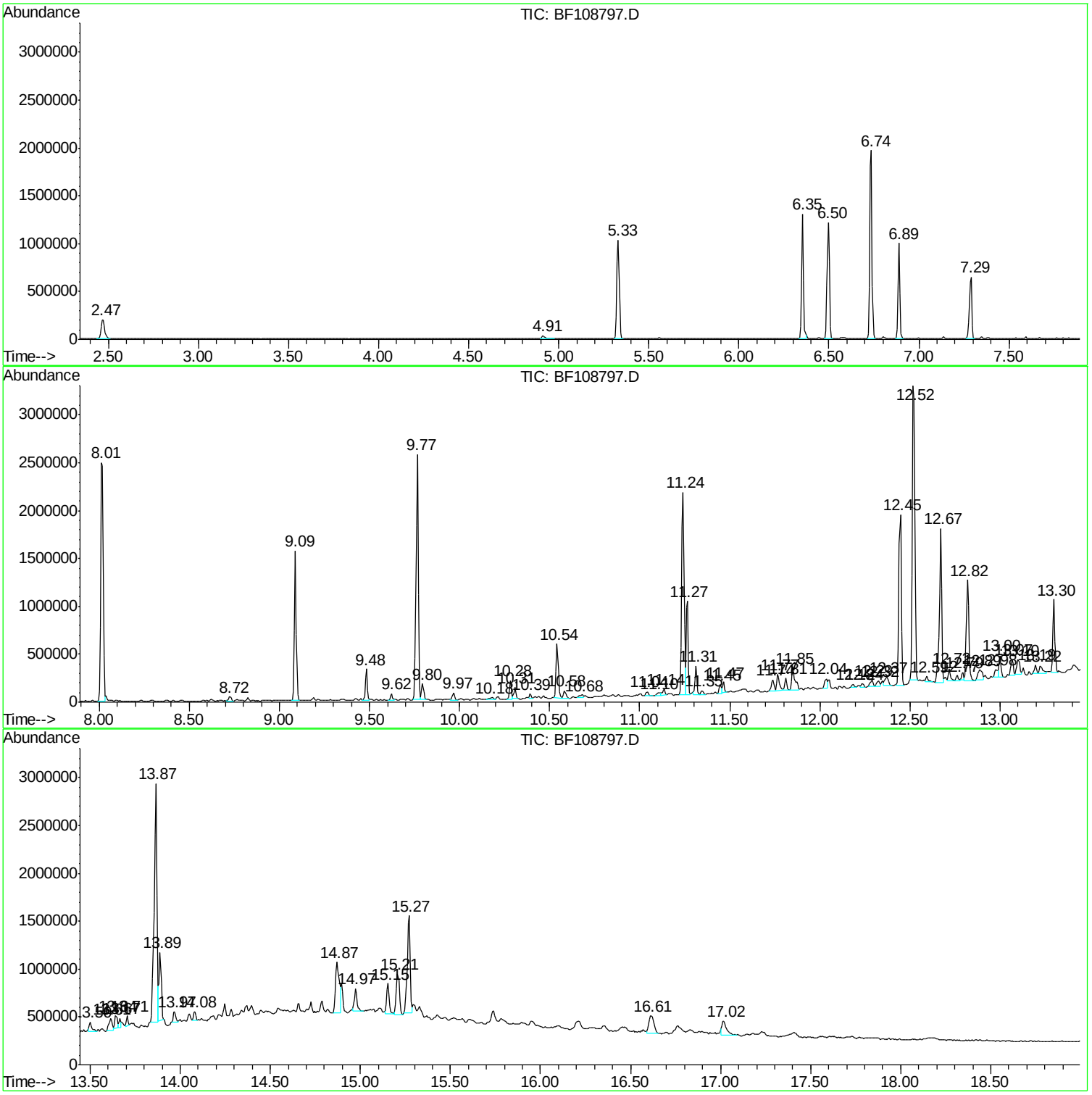
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DOCUMENTATION-#13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

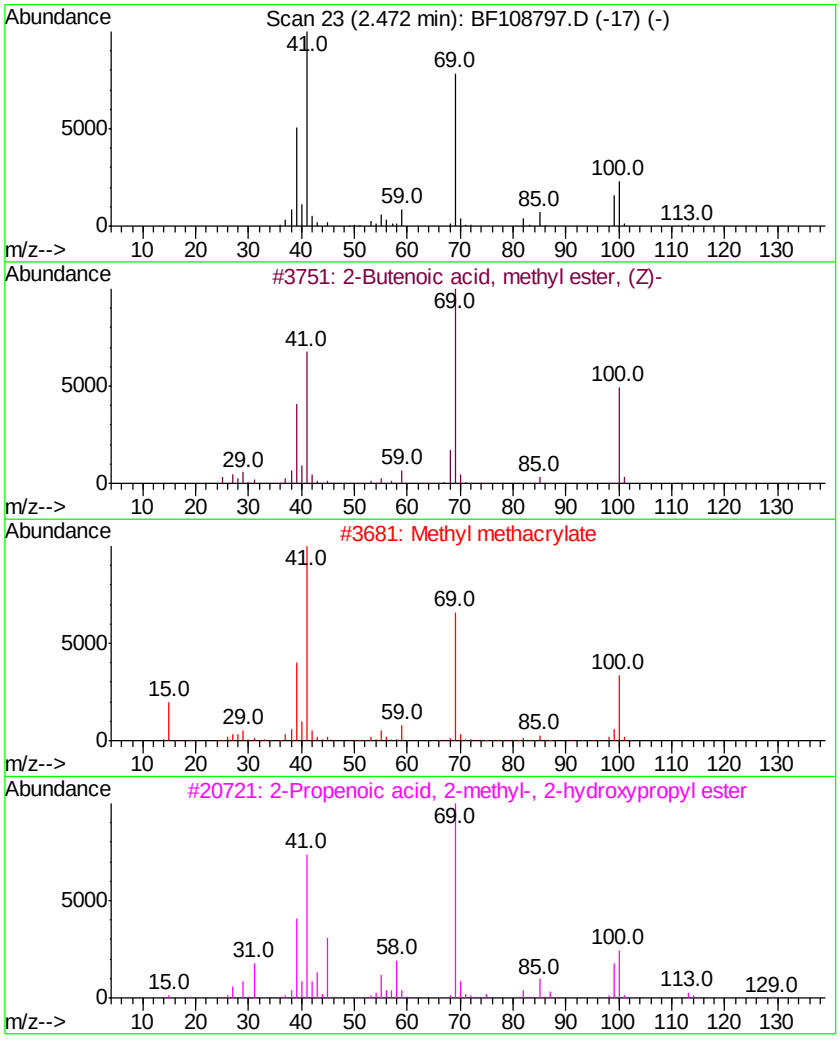
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

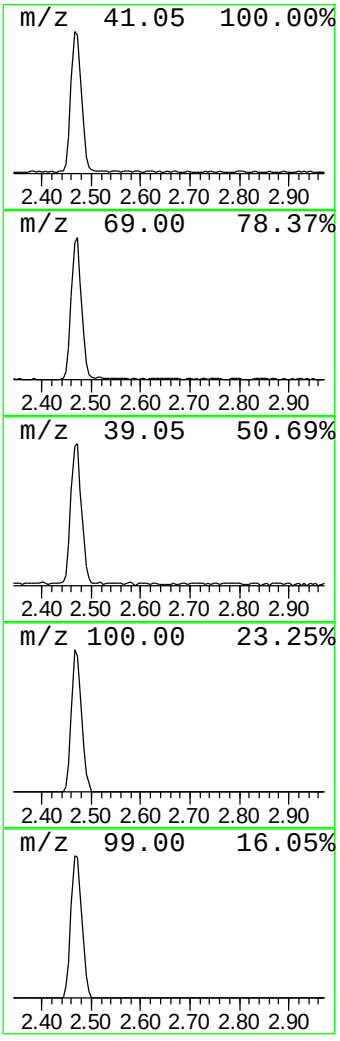
****

Peak Number 1 2-Butenoic acid, methyl est... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.47	3.29 ng	285789	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	83
2	Methyl methacrylate	100	C5H8O2	000080-62-6	80
3	2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	56
4	Methyl 3-butenoate	100	C5H8O2	003724-55-8	53
5	2-Butenoic acid, methyl ester, (E)-	100	C5H8O2	000623-43-8	42





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

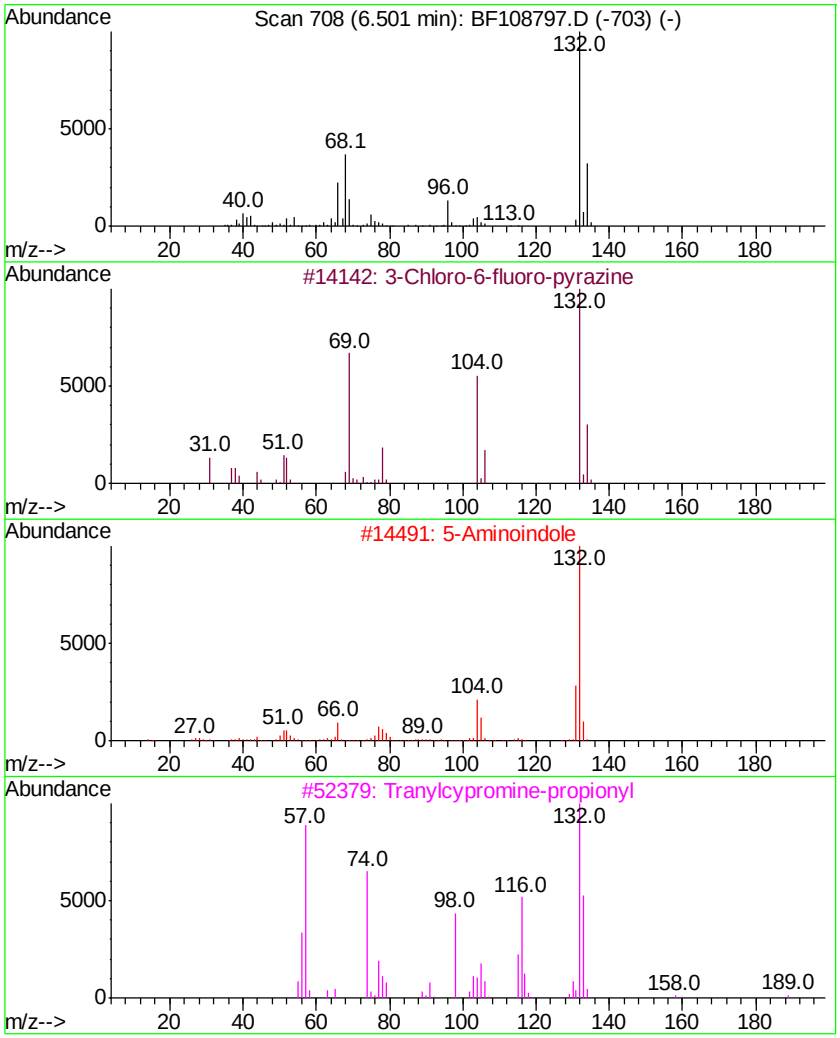
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

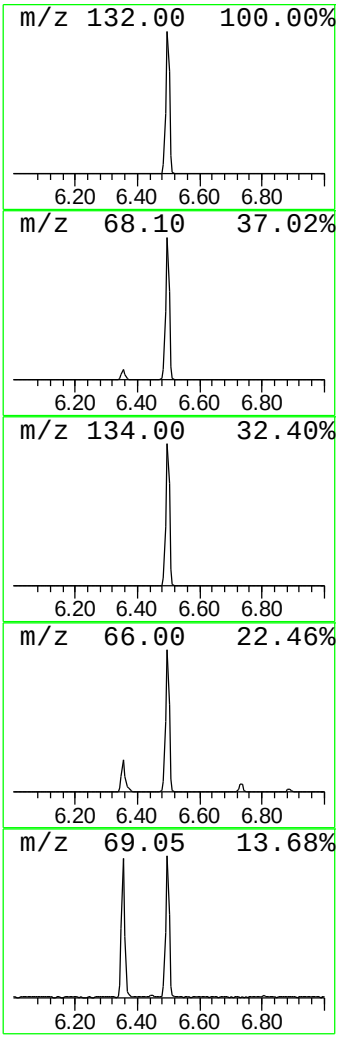
****

Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	11.37 ng	987196	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

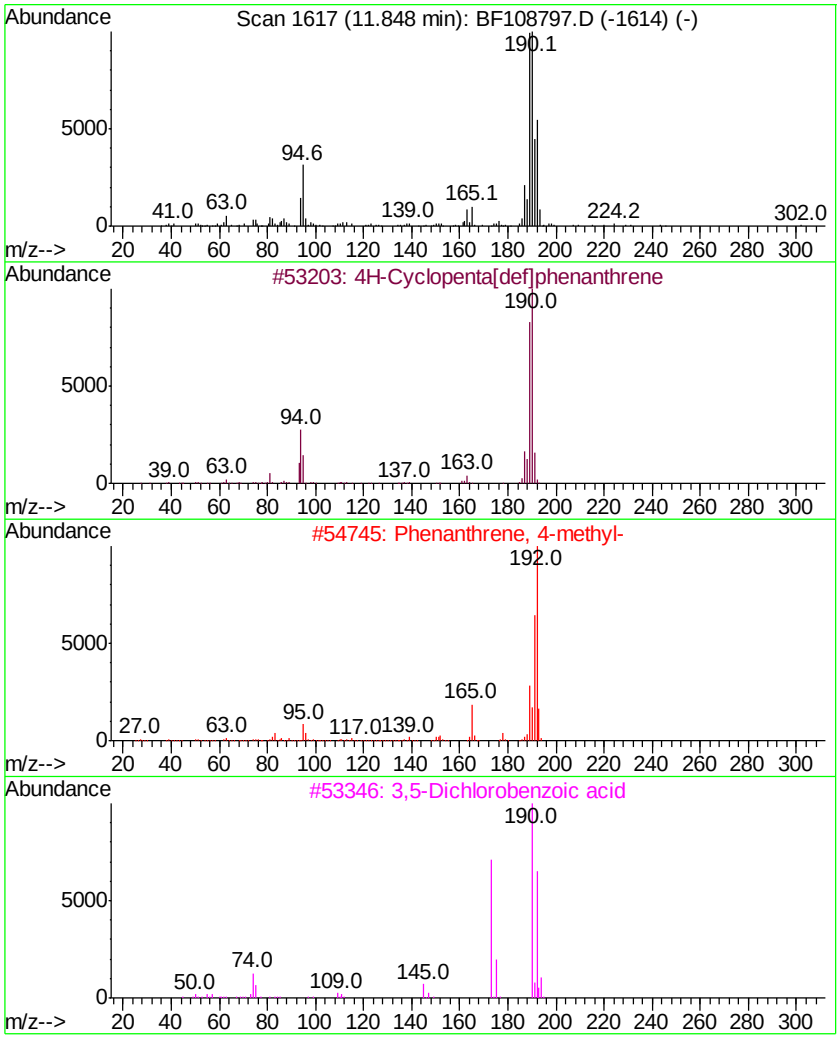
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

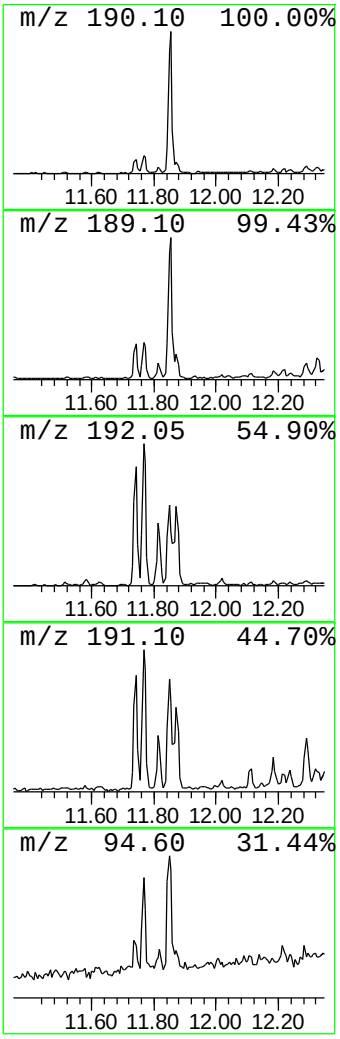
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	3.27 ng	312201	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	25
3	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	25
4	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	18
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

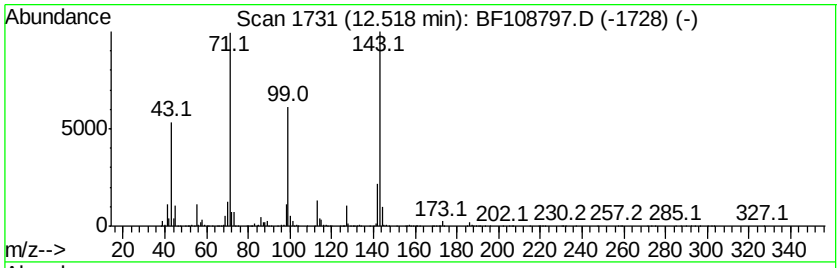
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

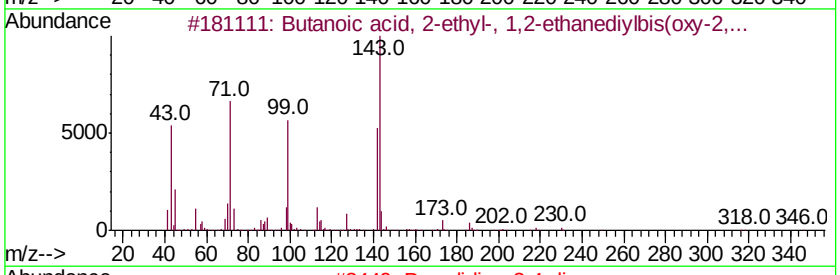
****

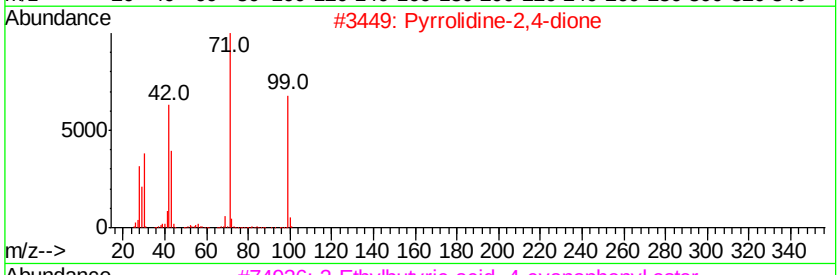
Peak Number 5 unknown12.52 Concentration Rank 1

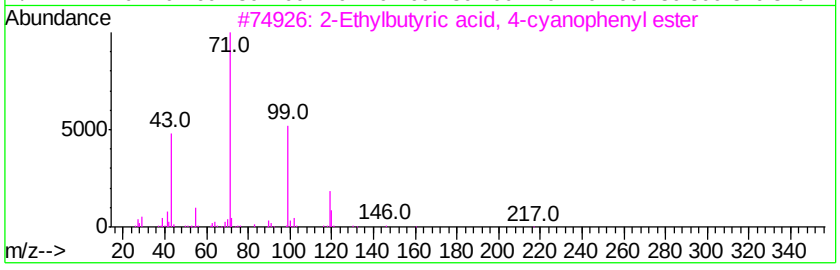
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	29.44 ng	2814640	Phenanthrene-d10	11.24

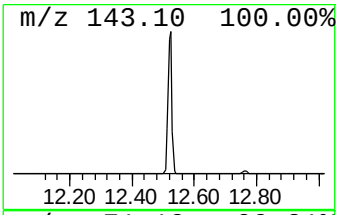
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-, 1,2-eth...	346	C18H34O6	000095-08-9	45
2	Pyrrolidine-2,4-dione	99	C4H5NO2	037772-89-7	38
3	2-Ethylbutyric acid, 4-cyanophen...	217	C13H15NO2	1000369-61-1	35
4	2-Ethylbutyric acid, 4-nitrophen...	237	C12H15NO4	1000369-85-5	35
5	Ethyl 3-ethoxyacrylate	144	C7H12O3	001001-26-9	35

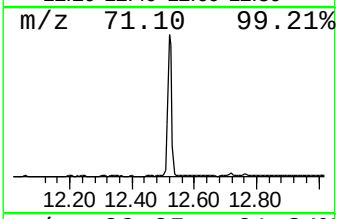


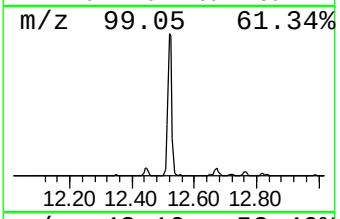


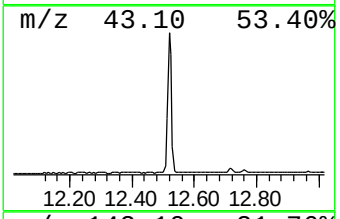


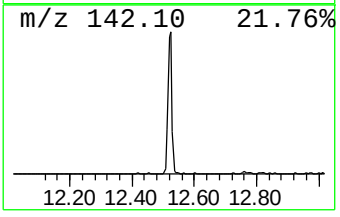












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090518\
Data File : BF108797.D
Acq On : 6 Sep 2018 1:44
Operator : JU/SJ
Sample : J4791-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-#13

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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
2-Butenoic acid, ...	2.47	3.3	ng	285789	1	6.74	1737000	20.0
unknown6.50	6.50	11.4	ng	987196	1	6.74	1737000	20.0
4H-Cyclopenta[def...	11.85	3.3	ng	312201	4	11.24	1911920	20.0
unknown12.52	12.52	29.4	ng	2814640	4	11.24	1911920	20.0