LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
Data File : BF108794.D
Acq On : 6 Sep 2018 00:22
Operator : JU/SJ
Sample : J4791-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-VST

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	4.931	438	441	448	rVB	140653	173172	3.97%	0.323%
2	5.342	506	511	514	rBV	4084076	4169649	95.48%	7.779%
3	6.366	680	685	688	rBV	4523752	4367056	100.00%	8.147%
4	6.501	704	708	712	rBV	4623052	4315023	98.81%	8.050%
5	6.566	716	719	726	rVB2	50603	58028	1.33%	0.108%
6	6.736	744	748	751	rBV	1824780	1482481	33.95%	2.766%
7	6.895	770	775	778	rBV	3617290	3401638	77.89%	6.346%
8	7.289	838	842	846	rBV	2587645	2557792	58.57%	4.772%
9	8.013	962	965	968	rBV	1934495	1731772	39.66%	3.231%
10	8.725	1083	1086	1090	rBV	54897	46507	1.06%	0.087%
11	9.095	1144	1149	1152	rBV	4702193	4351866	99.65%	8.119%
12	9.483	1211	1215	1218	rBV	1587419	1165751	26.69%	2.175%
13	9.625	1235	1239	1241	rBV	81484	65298	1.50%	0.122%
14	9.766	1259	1263	1266	rBV	1898767	1579943	36.18%	2.948%
15	9.795	1266	1268	1271	rVB	160590	116494	2.67%	0.217%
16	9.966	1294	1297	1301	rBV	97857	76645	1.76%	0.143%
17	10.307	1352	1355	1362	rVB	172585	139487	3.19%	0.260%
18	10.548	1392	1396	1399	rBV	2302842	2095941	47.99%	3.910%
19	10.854	1442	1448	1451	rBV3	33673	46919	1.07%	0.088%
20	11.042	1478	1480	1485	rVB	49879	48691	1.11%	0.091%
21	11.136	1492	1496	1499	rVB2	65435	60403	1.38%	0.113%
22	11.242	1510	1514	1516	rBV	1789979	1580875	36.20%	2.949%
23	11.266	1516	1518	1521	rVV	1300036	953251	21.83%	1.778%
24	11.313	1521	1526	1529	rVV	372696	311093	7.12%	0.580%
25	11.466	1547	1552	1555	rBV2	101790	116890	2.68%	0.218%
26	11.742	1596	1599	1601	rBV	152584	120438	2.76%	0.225%
27	11.771	1601	1604	1605	rBV	213850	225458	5.16%	0.421%
28	11.813	1608	1611	1614	rVB	696876	554574	12.70%	1.035%
29	11.848	1614	1617	1620	rBV	249500	291054	6.66%	0.543%
30	12.036	1646	1649	1650	rBV	132898	103720	2.38%	0.194%
31	12.289	1688	1692	1695	rBV	93195	116782	2.67%	0.218%
32	12.324	1695	1698	1700	rVV2	59670	67118	1.54%	0.125%
33	12.371	1703	1706	1711	rVB2	78021	108594	2.49%	0.203%
34	12.448	1715	1719	1722	rVB	1997879	1559723	35.72%	2.910%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : DOCUMENTATION-VST

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

35	12.501	1725	1728	1732	rBV3	39777	51992	1.19%	0.097%
36	12.542	1732	1735	1737	rVB	82737	73327	1.68%	0.137%
37	12.566	1737	1739	1742	rBV3	43905	62012	1.42%	0.116%
38	12.595	1742	1744	1749	rVB2	61205	68766	1.57%	0.128%
39	12.671	1752	1757	1760	rBV2	1515319	1658868	37.99%	3.095%
40	12.724	1763	1766	1772	rVB2	84853	104657	2.40%	0.195%
41	12.795	1775	1778	1779	rBV	107985	88992	2.04%	0.166%
42	12.824	1779	1783	1786	rVV	4568054	3898276	89.27%	7.273%
43	12.895	1790	1795	1798	rBV2	125537	212531	4.87%	0.397%
44	12.977	1806	1809	1811	rBV	92481	100776	2.31%	0.188%
45	13.001	1811	1813	1817	rVB	280546	234253	5.36%	0.437%
46	13.071	1821	1825	1827	rBV	184054	169302	3.88%	0.316%
47	13.107	1827	1831	1833	rBV	204050	200637	4.59%	0.374%
48	13.130	1833	1835	1838	rVB3	51449	54701	1.25%	0.102%
49	13.165	1838	1841	1843	rBV2	47237	51223	1.17%	0.096%
50	13.195	1844	1846	1849	rVB	97708	82803	1.90%	0.154%
51	13.224	1849	1851	1856	rBV2	100239	116356	2.66%	0.217%
52	13.501	1895	1898	1903	rVB	117549	131475	3.01%	0.245%
53	13.613	1913	1917	1920	rBV2	118663	171371	3.92%	0.320%
54	13.642	1920	1922	1924	rVV	130176	120543	2.76%	0.225%
55	13.665	1924	1926	1930	rVV2	111635	139925	3.20%	0.261%
56	13.707	1930	1933	1934	rVV2	103780	90257	2.07%	0.168%
57	13.730	1934	1937	1944	rVB	298533	324134	7.42%	0.605%
58	13.865	1955	1960	1962	rBV2	2093541	2495410	57.14%	4.656%
59	13.889	1962	1964	1967	rVB	750055	572313	13.11%	1.068%
60	13.971	1975	1978	1981	rBV	100153	95517	2.19%	0.178%
61	14.048	1989	1991	1994	rBV2	83182	79400	1.82%	0.148%
62	14.248	2023	2025	2028	rVB	132185	108864	2.49%	0.203%
63	14.283	2029	2031	2033	rVB	84943	63804	1.46%	0.119%
64	14.654	2092	2094	2099	rBV3	85714	111549	2.55%	0.208%
65	14.724	2103	2106	2109	rVB	488830	439710	10.07%	0.820%
66	14.871	2127	2131	2134	rBV	527712	778928	17.84%	1.453%
67	14.971	2145	2148	2154	rVB	215192	242131	5.54%	0.452%
68	15.154	2176	2179	2184	rVB	281235	315217	7.22%	0.588%
69	15.207	2185	2188	2192	rVB	442624	467024	10.69%	0.871%
70	15.265	2194	2198	2202	rBV	929166	1142234	26.16%	2.131%
71	16.612	2424	2427	2434	rVB3	173810	321086	7.35%	0.599%

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Misc :
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Instrument :
BNA_F
ClientSampleId :
DOCUMENTATION-VST

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 53600490

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
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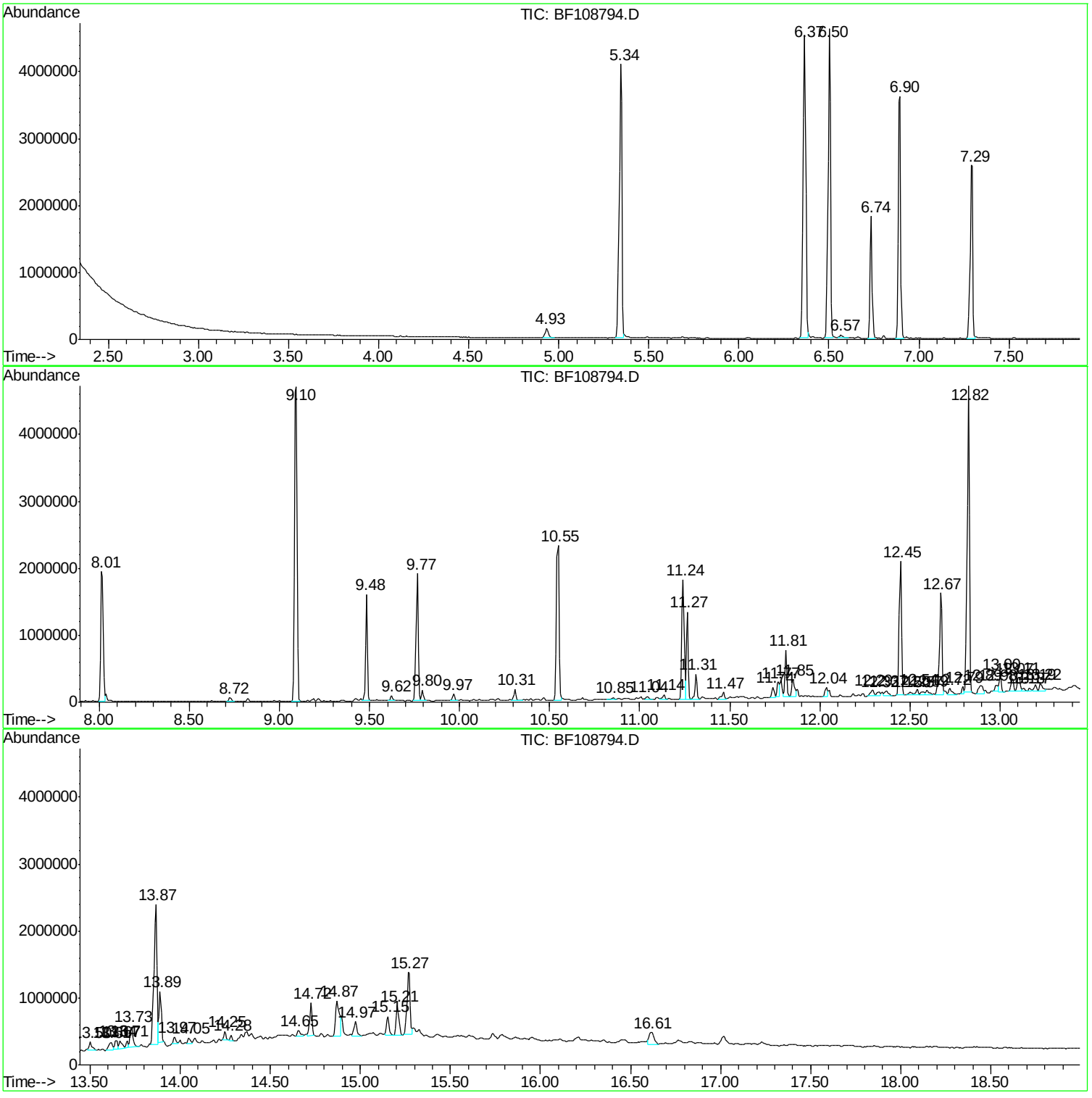
Sample : J4791-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-VST

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 : BF108794.D
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Instrument : BNA_F
ClientSampleId : DOCUMENTATION-VST

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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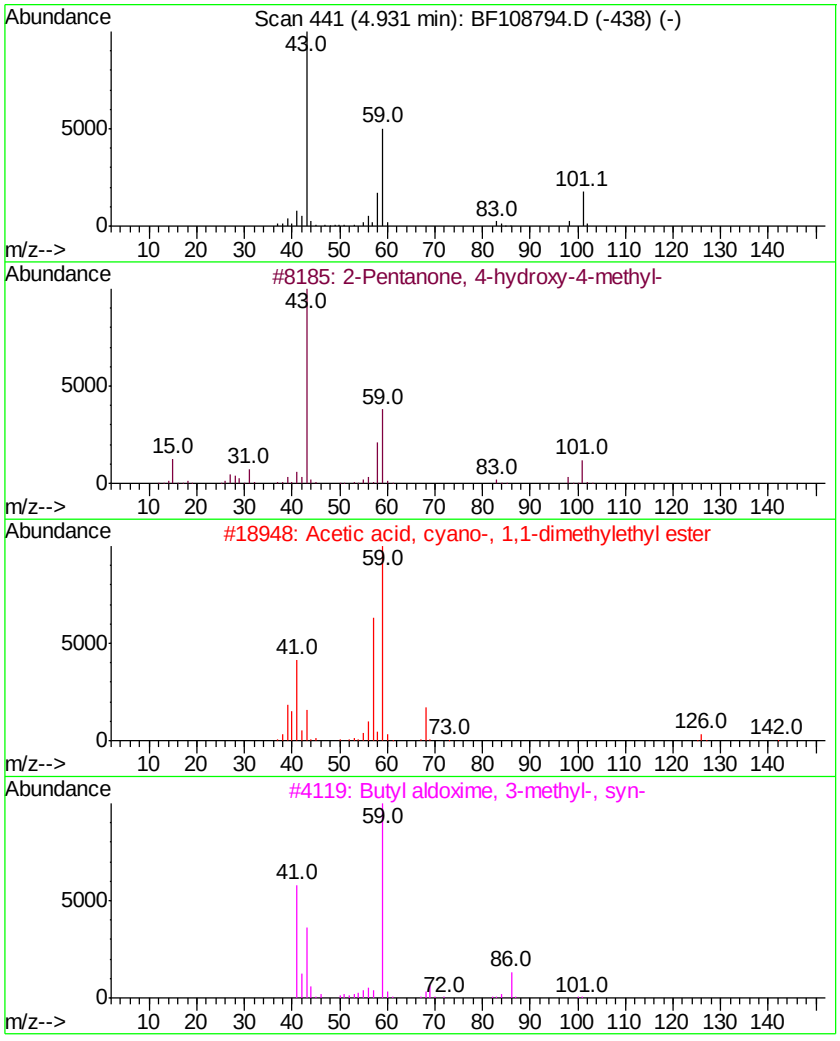
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

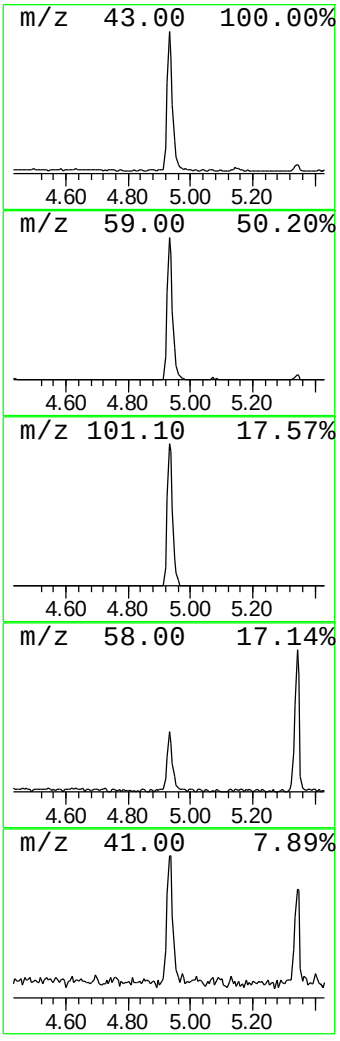
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.34 ng	173172	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	Acetone	58	C3H6O	000067-64-1	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090518\
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Sample : J4791-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DOCUMENTATION-VST

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

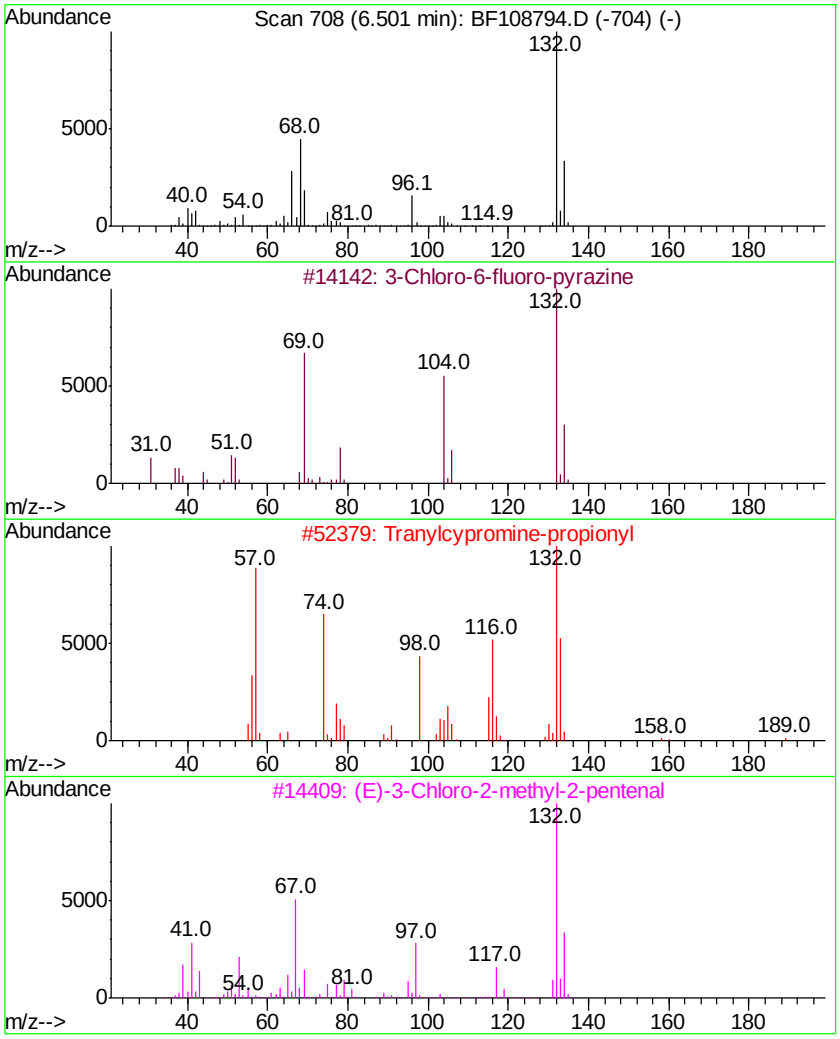
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

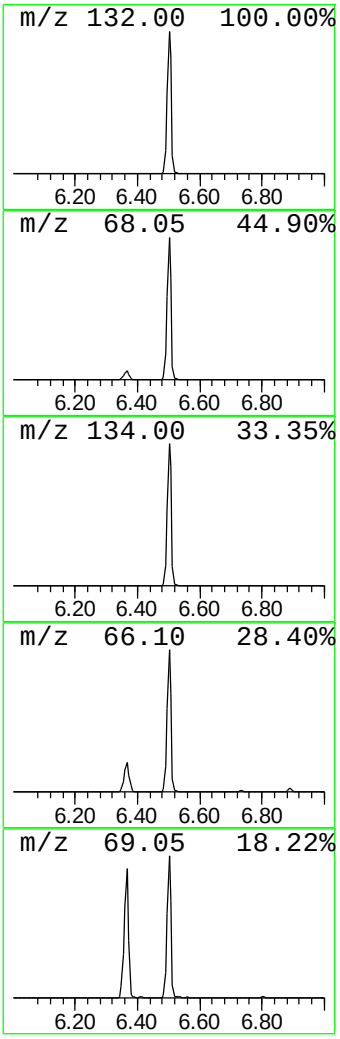
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	58.21 ng	4315020	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Sample : J4791-01
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Instrument : BNA_F
ClientSampleId : DOCUMENTATION-VST

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
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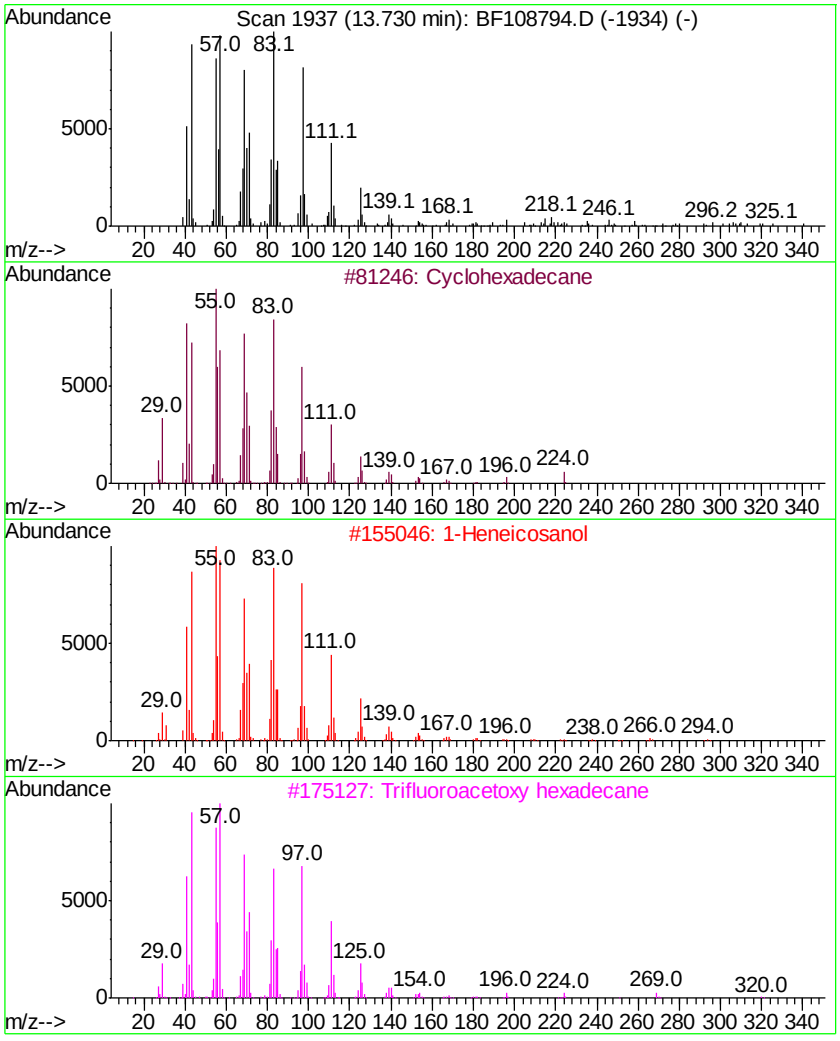
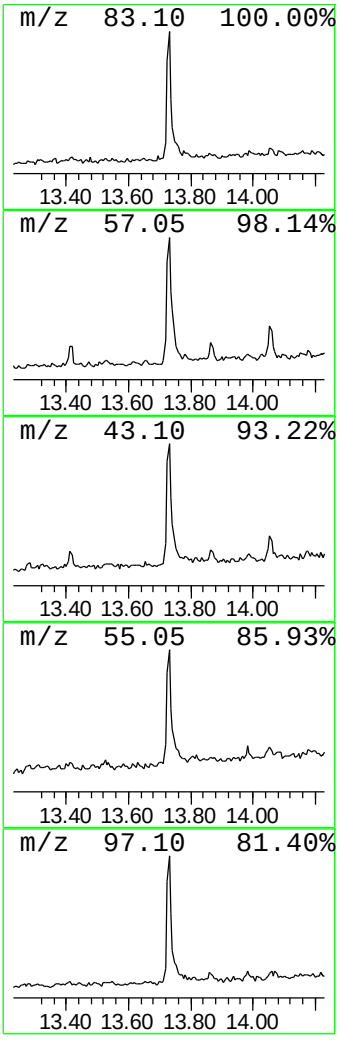
Peak Number 4 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.60 ng	324134	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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

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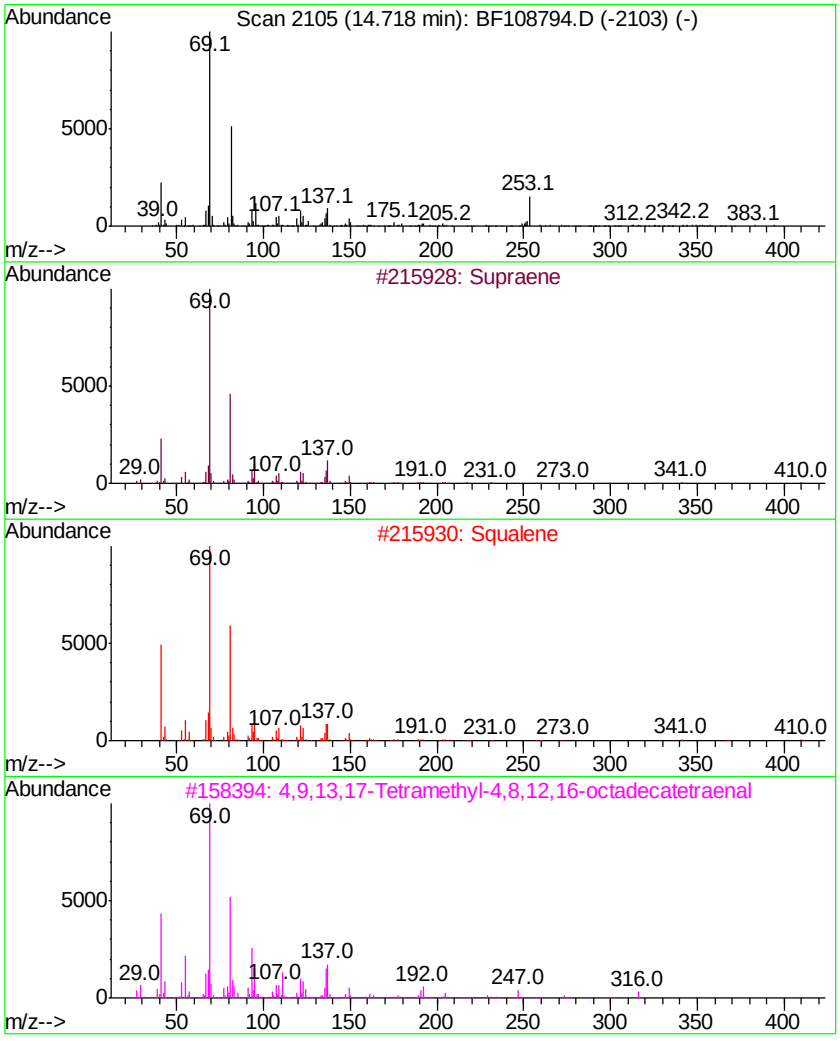
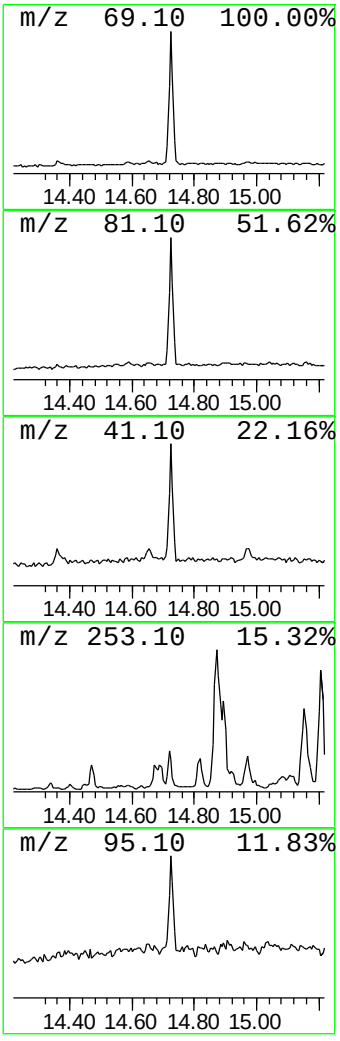
Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	7.70 ng	439710	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	Squalene	410	C30H50	000111-02-4	90
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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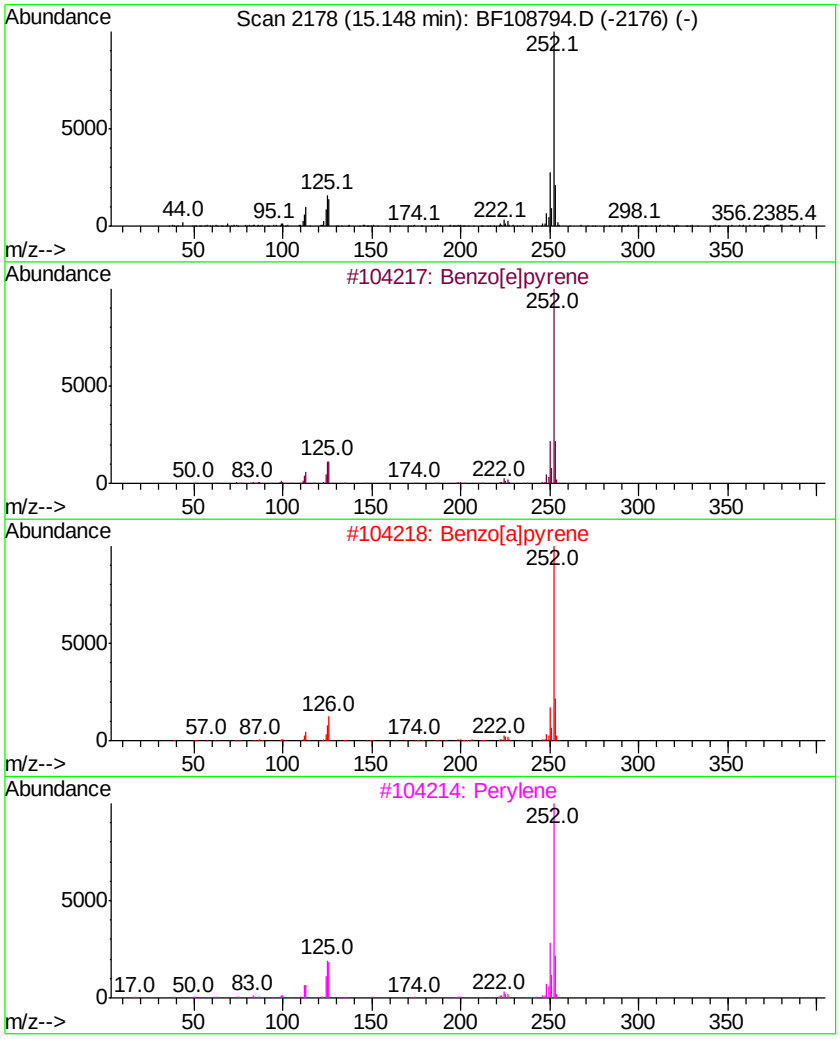
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

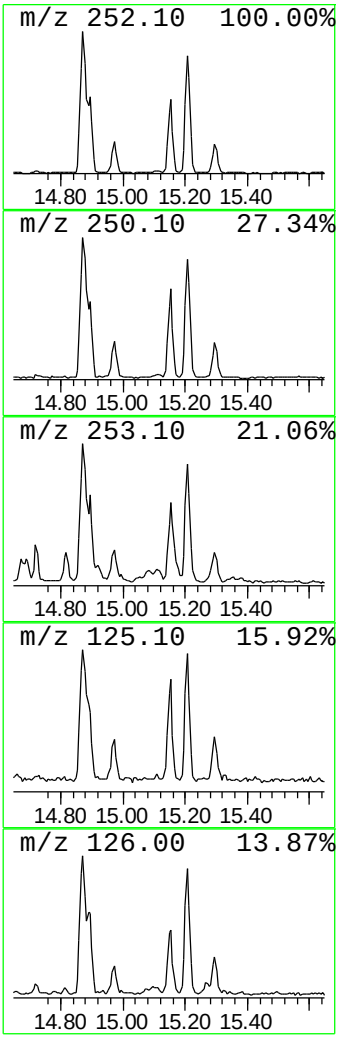
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	5.52 ng	315217	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93





Tentatively Identified Compound (LSC) summary

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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-Pentanone, 4-hy...	4.93	2.3	ng	173172	1	6.74	1482480	20.0
unknown6.50	6.50	58.2	ng	4315020	1	6.74	1482480	20.0
Cyclohexadecane	13.73	2.6	ng	324134	5	13.87	2495410	20.0
Supraene	14.72	7.7	ng	439710	6	15.27	1142230	20.0
Benzo[e]pyrene	15.15	5.5	ng	315217	6	15.27	1142230	20.0