LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000697.D
Acq On : 13 Oct 2019 03:16
Operator : JU
Sample : K5348-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190830-COMPOSITE-F

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_P\METHODS\8270-BP100119.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	4.946	482	486	490	rBV	1066843	1095466	25.74%	2.731%
2	5.375	555	559	575	rVB	1096993	1075792	25.28%	2.682%
3	6.293	712	715	720	rBV	180741	181120	4.26%	0.452%
4	6.393	728	732	743	rBV	3248207	3233443	75.97%	8.061%
5	6.522	750	754	757	rBV	2648177	2141428	50.31%	5.338%
6	6.752	789	793	796	rBV	1394281	1189528	27.95%	2.965%
7	6.816	801	804	812	rBV	106061	90692	2.13%	0.226%
8	6.905	815	819	823	rBV	3823913	3171132	74.51%	7.905%
9	7.311	884	888	891	rBV	2760863	2265390	53.23%	5.647%
10	7.528	921	925	928	rVB	166933	140467	3.30%	0.350%
11	7.940	986	995	999	rBV6	27517	60367	1.42%	0.150%
12	8.034	1007	1011	1014	rBV	1799555	1482377	34.83%	3.695%
13	8.675	1116	1120	1126	rBV2	48239	61698	1.45%	0.154%
14	8.752	1126	1133	1136	rBV5	39192	54982	1.29%	0.137%
15	9.116	1191	1195	1198	rBV	4948299	3996210	93.89%	9.962%
16	9.205	1205	1210	1211	rBV3	48648	71491	1.68%	0.178%
17	9.510	1259	1262	1267	rBV	850108	670631	15.76%	1.672%
18	9.657	1283	1287	1292	rBV	135277	155566	3.66%	0.388%
19	9.710	1294	1296	1299	rVB2	65367	58914	1.38%	0.147%
20	9.799	1307	1311	1314	rVB	2068129	1783993	41.92%	4.447%
21	10.046	1350	1353	1355	rVB	75777	65328	1.53%	0.163%
22	10.346	1402	1404	1410	rVB2	41291	57995	1.36%	0.145%
23	10.587	1442	1445	1451	rBV	517307	492274	11.57%	1.227%
24	10.716	1464	1467	1468	rBV	74774	64763	1.52%	0.161%
25	10.781	1475	1478	1481	rBV	56859	65883	1.55%	0.164%
26	10.957	1505	1508	1513	rBV4	68495	71010	1.67%	0.177%
27	11.022	1516	1519	1521	rBV	114971	105222	2.47%	0.262%
28	11.157	1538	1542	1546	rBV	438213	418438	9.83%	1.043%
29	11.293	1561	1565	1568	rBV	2291945	1943215	45.66%	4.844%
30	11.316	1568	1569	1572	rVV	295003	173214	4.07%	0.432%
31	11.363	1574	1577	1581	rVB3	243182	252034	5.92%	0.628%
32	11.528	1602	1605	1608	rBV	106853	96738	2.27%	0.241%
33	11.798	1649	1651	1654	rVB	59804	55287	1.30%	0.138%
34	11.834	1654	1657	1660	rBV2	86008	101955	2.40%	0.254%

LSC Area Percent Report

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Misc :
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Instrument : BNA_P
ClientSampleId : 20190830-COMPOSITE-F

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_P\METHODS\8270-BP100119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.916	1669	1671	1673	rVB	111283	86436	2.03%	0.215%
36	12.093	1699	1701	1704	rVB3	78431	76434	1.80%	0.191%
37	12.357	1744	1746	1749	rBV2	106240	98608	2.32%	0.246%
38	12.440	1758	1760	1762	rBV2	88642	103670	2.44%	0.258%
39	12.522	1770	1774	1777	rBV	800731	741211	17.41%	1.848%
40	12.616	1788	1790	1793	rBV	106080	109684	2.58%	0.273%
41	12.751	1808	1813	1816	rBV	835451	802367	18.85%	2.000%
42	12.898	1835	1838	1842	rBV	4799069	4256190	100.00%	10.610%
43	13.087	1868	1870	1873	rVB	261779	218469	5.13%	0.545%
44	13.151	1879	1881	1883	rVB	192337	144367	3.39%	0.360%
45	13.816	1991	1994	2001	rBV2	483653	599231	14.08%	1.494%
46	13.969	2015	2020	2023	rBV2	2105873	2685686	63.10%	6.695%
47	13.993	2023	2024	2027	rVB	430884	243172	5.71%	0.606%
48	15.022	2196	2199	2206	rVB	537975	1020933	23.99%	2.545%
49	15.381	2258	2260	2263	rBV	365254	388475	9.13%	0.968%
50	15.451	2268	2272	2275	rBV	1346832	1595258	37.48%	3.977%

Sum of corrected areas: 40114234

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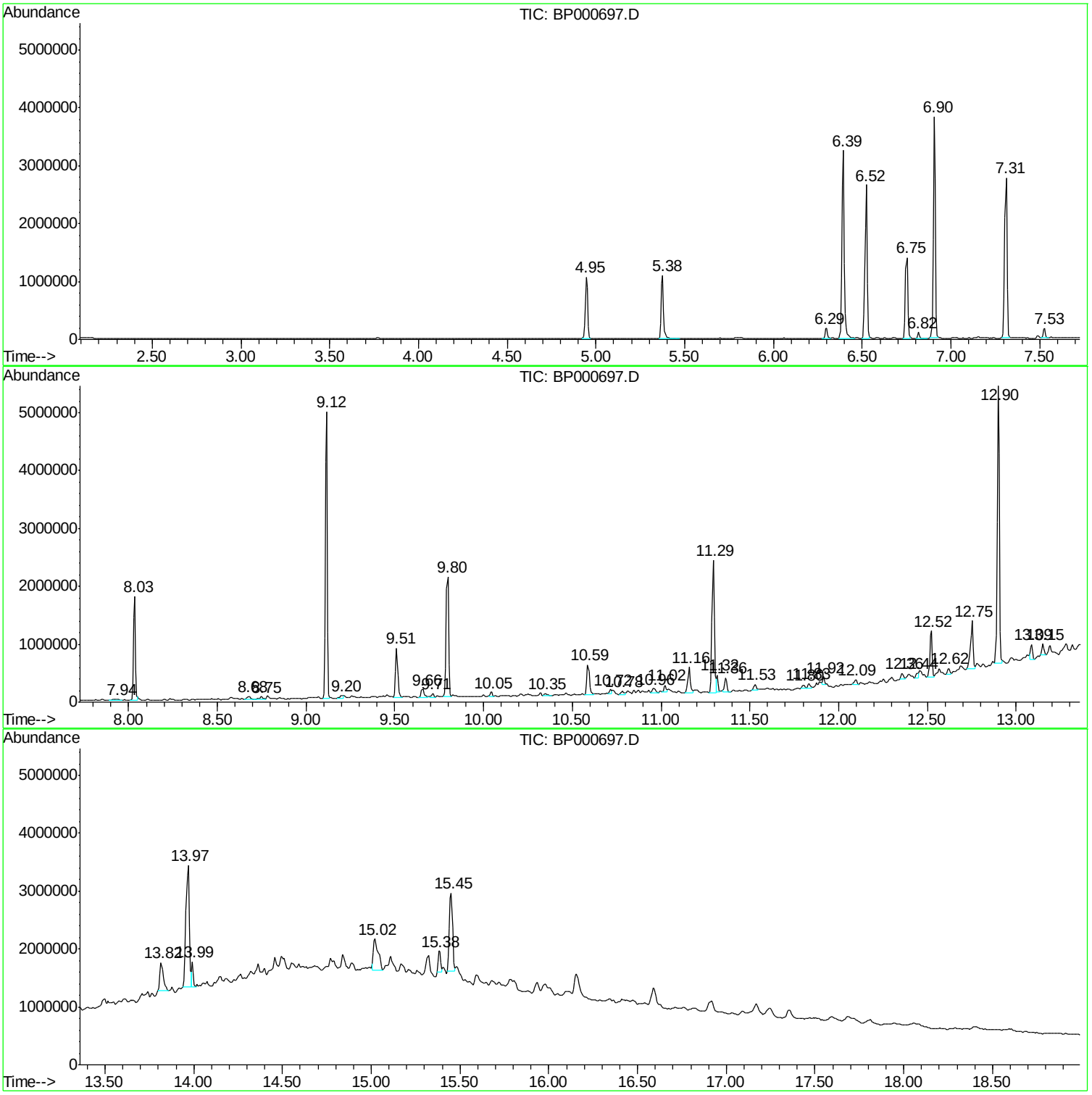
Instrument : BNA_P
ClientSampleId : 20190830-COMPOSITE-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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 P\DATA\BP101319\
Data File : BP000697.D
Acq On : 13 Oct 2019 03:16
Operator : JU
Sample : K5348-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190830-COMPOSITE-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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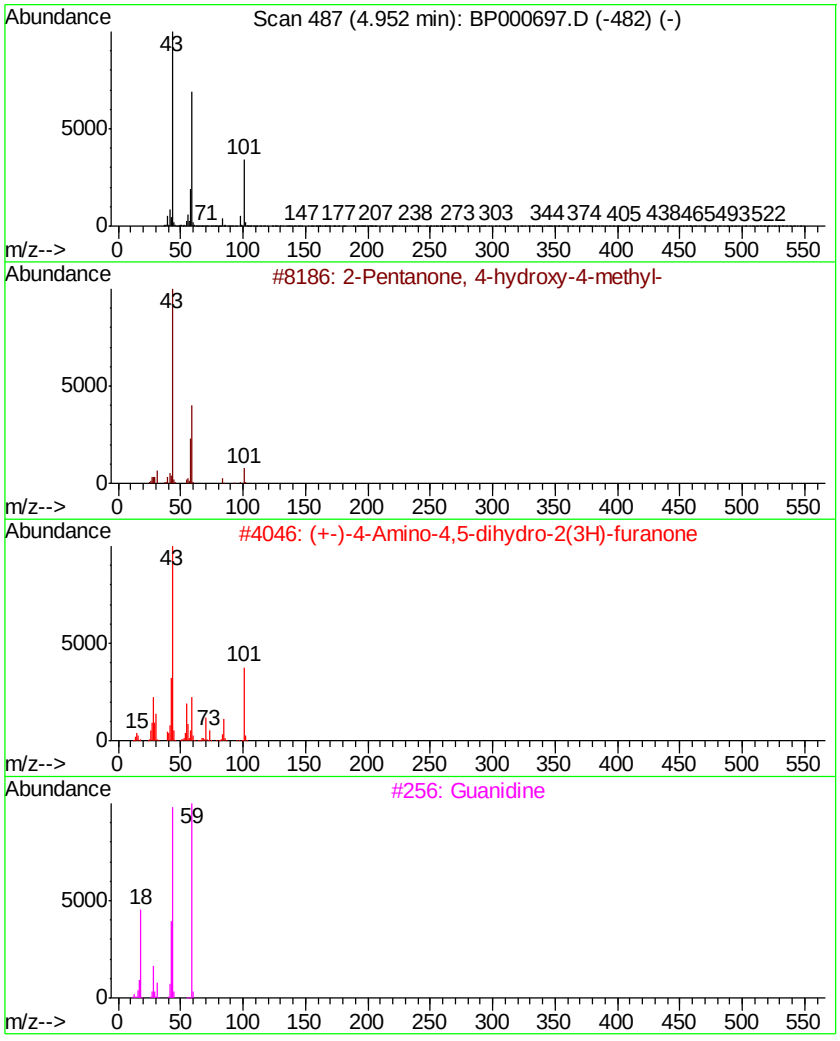
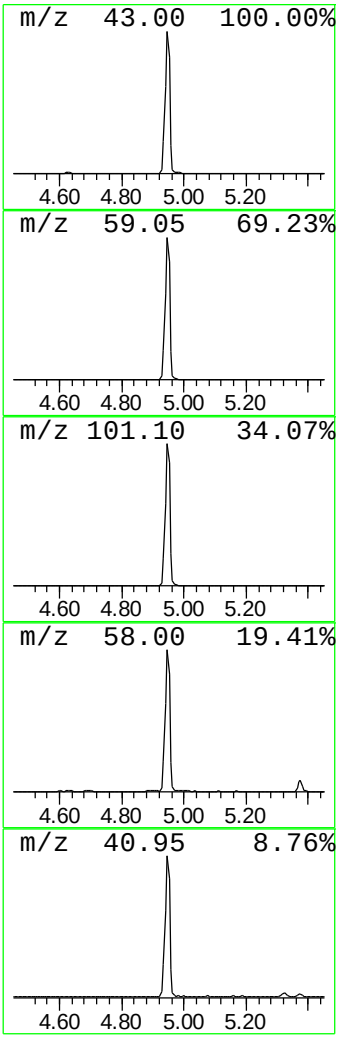
Peak Number 1 unknown4.95 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	18.42 ng	1095470	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Guanidine	59	CH5N3	000113-00-8	38
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument : BNA_P
ClientSampleId : 20190830-COMPOSITE-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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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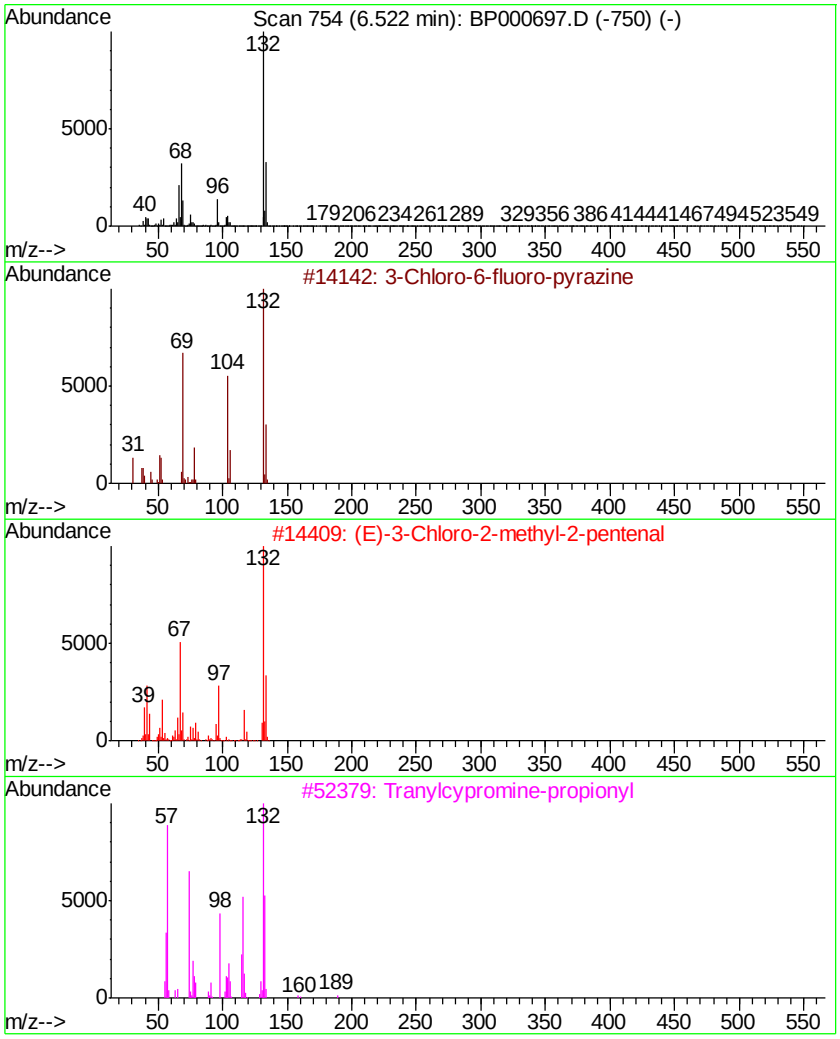
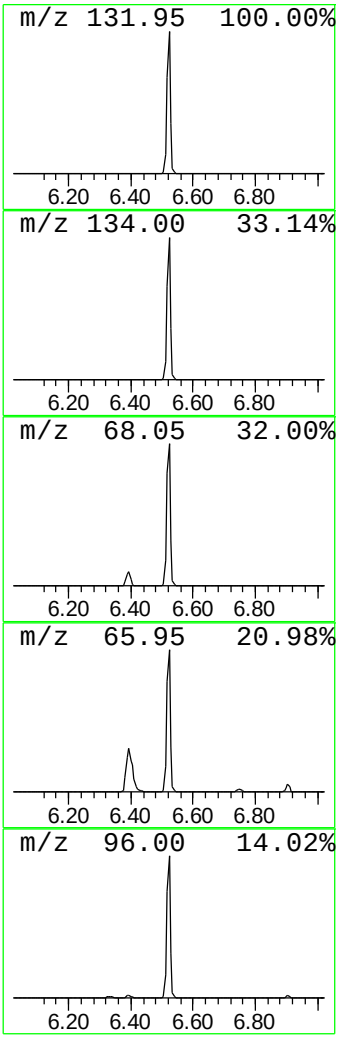
Peak Number 2 unknown6.52 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	36.00 ng	2141430	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Acq On : 13 Oct 2019 03:16
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Instrument : BNA_P
ClientSampleId : 20190830-COMPOSITE-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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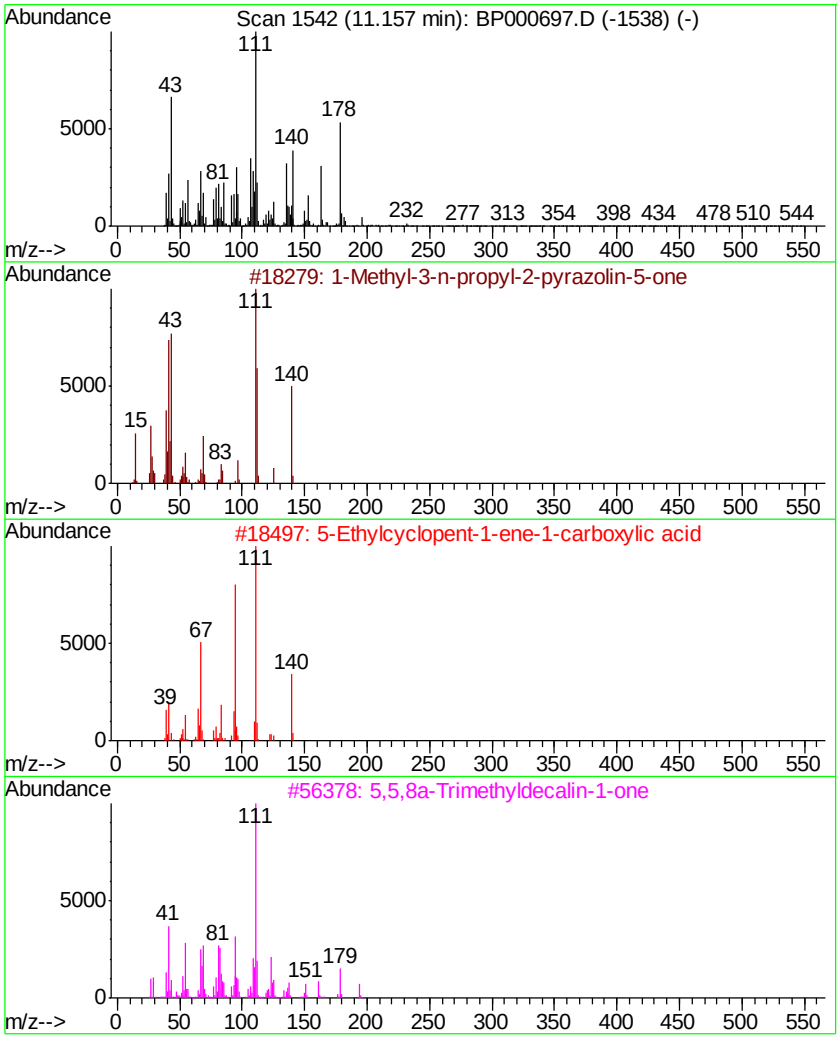
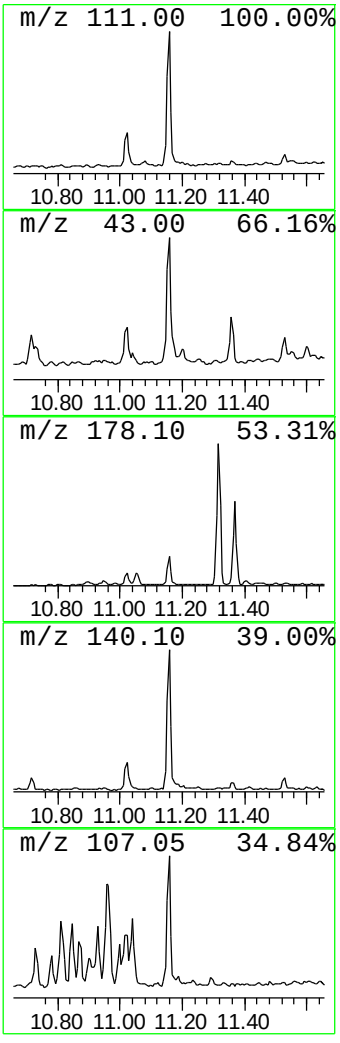
Peak Number 4 unknown11.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	4.31 ng	418438	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-3-n-propyl-2-pyrazolin-...	140	C7H12N2O	031272-04-5	27
2	5-Ethylcyclopent-1-ene-1-carboxy...	140	C8H12O2	036258-07-8	27
3	5,5,8a-Trimethyldecalin-1-one	194	C13H22O	1000195-96-1	25
4	4-Pyridinol-1-oxide	111	C5H5NO2	006890-62-6	22
5	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	22





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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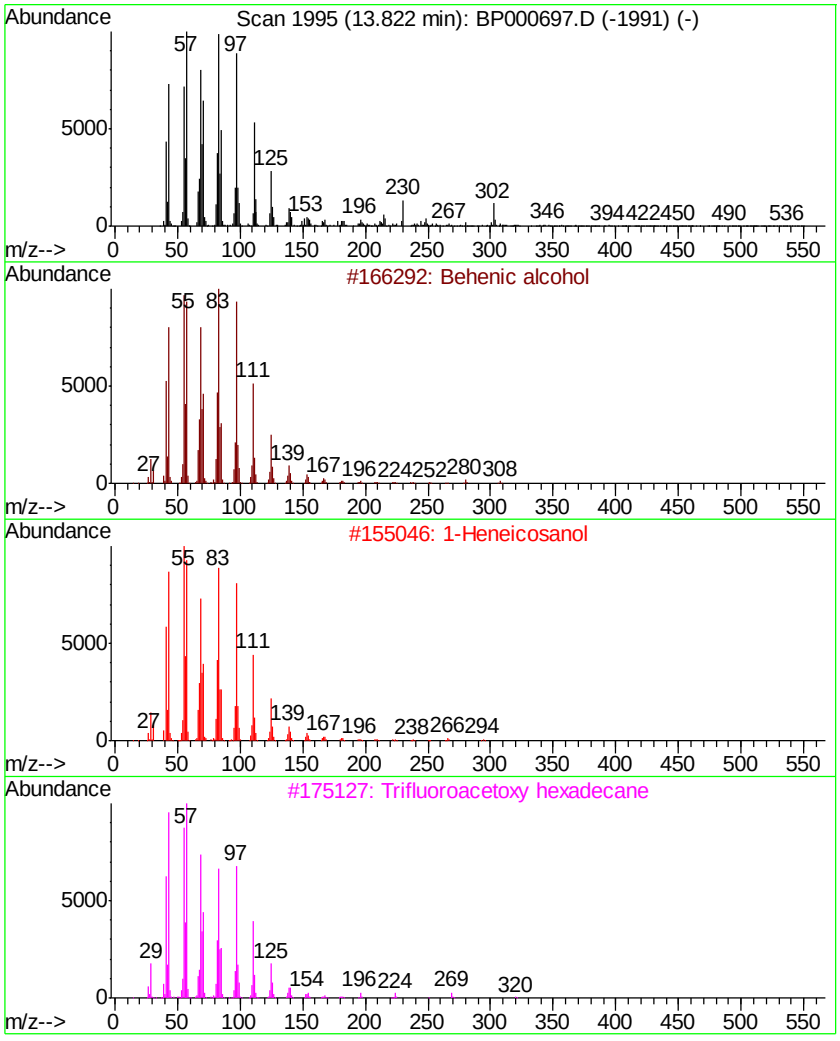
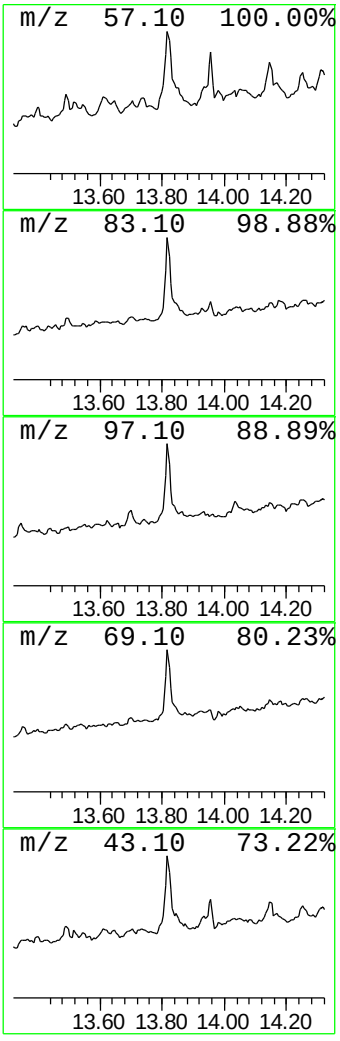
Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.46 ng	599231	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





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
unknown4.95	4.95	18.4	ng	1095470	1	6.75	1189530	20.0
unknown6.52	6.52	36.0	ng	2141430	1	6.75	1189530	20.0
unknown11.16	11.16	4.3	ng	418438	4	11.29	1943220	20.0
Behenic alcohol	13.82	4.5	ng	599231	5	13.97	2685690	20.0