LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112216.D
Acq On : 24 Jan 2019 18:38
Operator : JU/SJ
Sample : K1223-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-P

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-BF011619.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	5.057	502	505	512	rBV	82844	93636	4.20%	0.314%
2	5.487	574	578	593	rBV	2023066	1942440	87.10%	6.511%
3	6.498	746	750	765	rBV	2025254	1869988	83.86%	6.268%
4	6.628	769	772	782	rVV	1974629	1758289	78.85%	5.893%
5	6.857	807	811	817	rBV	1095440	981311	44.00%	3.289%
6	7.010	833	837	841	rBV	1583838	1323814	59.36%	4.437%
7	7.416	902	906	917	rVB	1304572	1253060	56.19%	4.200%
8	8.139	1025	1029	1031	rBV	1670800	1473002	66.05%	4.937%
9	8.157	1031	1032	1041	rVB	164601	136685	6.13%	0.458%
10	8.851	1147	1150	1153	rBV	49220	44333	1.99%	0.149%
11	8.951	1164	1167	1171	rBV2	38639	42145	1.89%	0.141%
12	9.210	1207	1211	1221	rBV	2630359	2230020	100.00%	7.474%
13	9.292	1221	1225	1227	rVV3	29821	30514	1.37%	0.102%
14	9.363	1233	1237	1242	rVB8	33724	49991	2.24%	0.168%
15	9.481	1253	1257	1262	rBV5	25667	40310	1.81%	0.135%
16	9.528	1262	1265	1266	rBV3	47586	38087	1.71%	0.128%
17	9.551	1266	1269	1272	rVV	375279	296721	13.31%	0.995%
18	9.604	1275	1278	1282	rVB	215065	206980	9.28%	0.694%
19	9.651	1282	1286	1288	rBV2	86618	86130	3.86%	0.289%
20	9.751	1301	1303	1307	rBV4	20171	30762	1.38%	0.103%
21	9.804	1310	1312	1314	rBV2	39707	29012	1.30%	0.097%
22	9.892	1321	1327	1330	rBV2	1797449	1675771	75.15%	5.617%
23	9.922	1330	1332	1336	rVB2	209748	194139	8.71%	0.651%
24	9.963	1337	1339	1342	rVB2	42223	42176	1.89%	0.141%
25	10.016	1342	1348	1352	rBV4	183052	270529	12.13%	0.907%
26	10.098	1359	1362	1365	rVB2	101964	90323	4.05%	0.303%
27	10.186	1374	1377	1379	rBV2	61456	47615	2.14%	0.160%
28	10.322	1394	1400	1403	rBV3	38611	57833	2.59%	0.194%
29	10.439	1417	1420	1425	rBV	123206	109207	4.90%	0.366%
30	10.533	1433	1436	1439	rBV4	82241	79121	3.55%	0.265%
31	10.563	1439	1441	1444	rVB2	96140	85437	3.83%	0.286%
32	10.598	1444	1447	1448	rBV2	34502	30078	1.35%	0.101%
33	10.681	1458	1461	1465	rBV	1274040	1248457	55.98%	4.184%
34	10.804	1478	1482	1488	rVB4	100985	153681	6.89%	0.515%

LSC Area Percent Report

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Sample : K1223-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-P

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-BF011619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.039	1520	1522	1525	rBV4	31830	35019	1.57%	0.117%
36	11.098	1529	1532	1534	rBV3	34115	34674	1.55%	0.116%
37	11.186	1544	1547	1550	rBV2	39209	37531	1.68%	0.126%
38	11.275	1560	1562	1568	rVB2	84132	86916	3.90%	0.291%
39	11.380	1576	1580	1582	rBV	1658942	1425166	63.91%	4.777%
40	11.404	1582	1584	1587	rVV	955089	779917	34.97%	2.614%
41	11.428	1587	1588	1590	rVV	136138	93384	4.19%	0.313%
42	11.457	1590	1593	1596	rVV	236846	196983	8.83%	0.660%
43	11.492	1596	1599	1600	rVV2	39470	42524	1.91%	0.143%
44	11.516	1600	1603	1605	rVB	97324	78499	3.52%	0.263%
45	11.592	1613	1616	1617	rBV3	48617	51289	2.30%	0.172%
46	11.610	1617	1619	1623	rVB	84636	89055	3.99%	0.298%
47	11.722	1635	1638	1642	rBV2	95581	109300	4.90%	0.366%
48	11.869	1659	1663	1664	rBV	207554	207398	9.30%	0.695%
49	11.904	1667	1669	1676	rVB2	364349	418328	18.76%	1.402%
50	11.998	1681	1685	1687	rBV	127085	146669	6.58%	0.492%
51	12.075	1696	1698	1703	rVB4	131656	119242	5.35%	0.400%
52	12.204	1718	1720	1723	rVB2	70727	67643	3.03%	0.227%
53	12.263	1728	1730	1733	rVB4	54665	42448	1.90%	0.142%
54	12.310	1735	1738	1739	rBV2	54236	59918	2.69%	0.201%
55	12.357	1743	1746	1748	rBV2	67910	75759	3.40%	0.254%
56	12.516	1770	1773	1778	rBV	532573	501870	22.51%	1.682%
57	12.598	1783	1787	1791	rBV	1002436	978891	43.90%	3.281%
58	12.686	1800	1802	1806	rBV5	78582	93693	4.20%	0.314%
59	12.827	1820	1826	1832	rVB	809264	906354	40.64%	3.038%
60	12.963	1845	1849	1852	rBV	1903052	1595309	71.54%	5.347%
61	13.392	1920	1922	1926	rVB2	287783	275359	12.35%	0.923%
62	13.857	1998	2001	2007	rVB2	256477	314711	14.11%	1.055%
63	14.027	2025	2030	2032	rBV2	1403453	1548919	69.46%	5.192%
64	14.051	2032	2034	2037	rVB	333992	251393	11.27%	0.843%
65	15.127	2215	2217	2220	rBV	263897	229231	10.28%	0.768%
66	15.510	2278	2282	2286	rBV	714310	900353	40.37%	3.018%

Sum of corrected areas: 29835342

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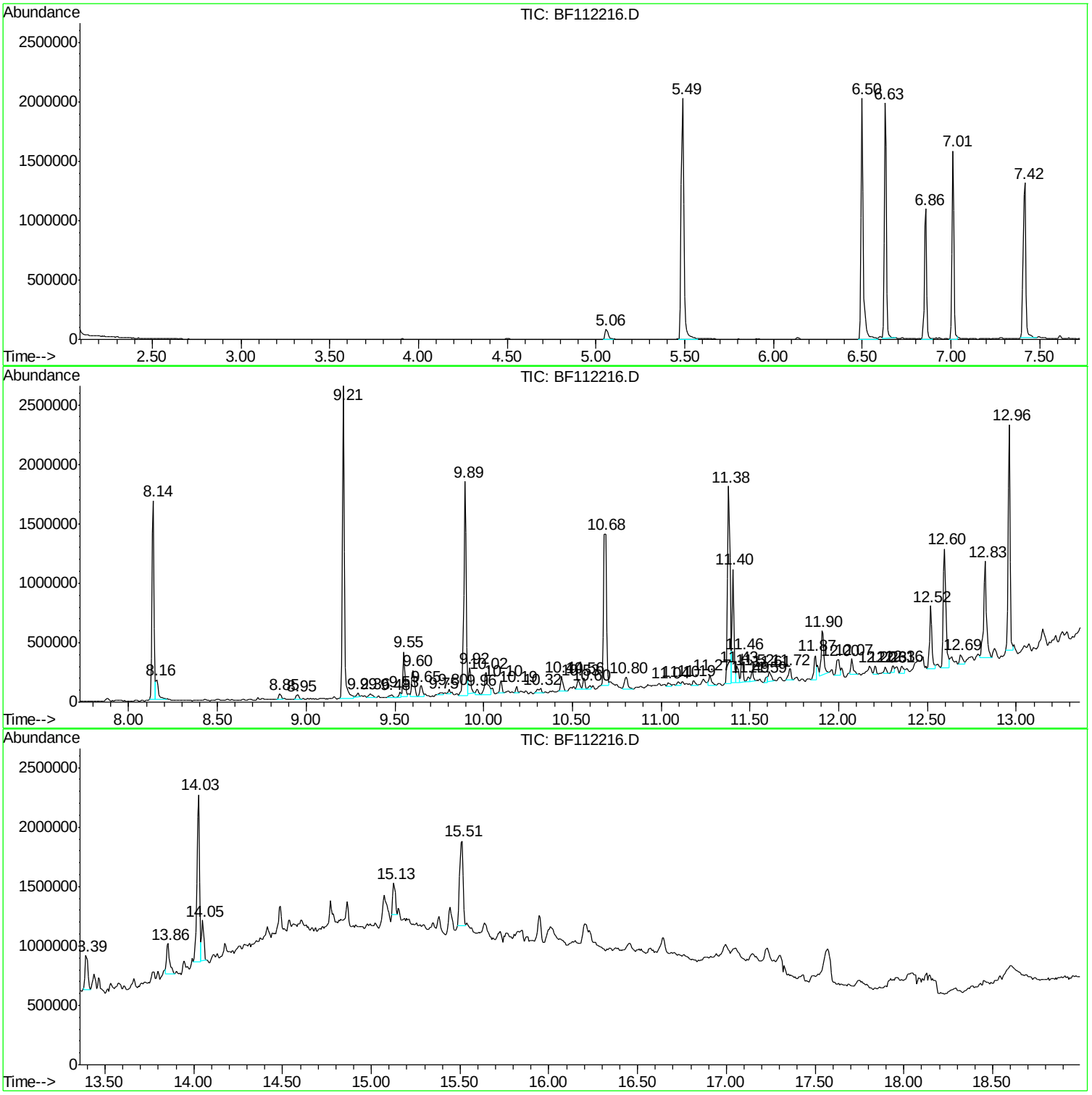
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-P

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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

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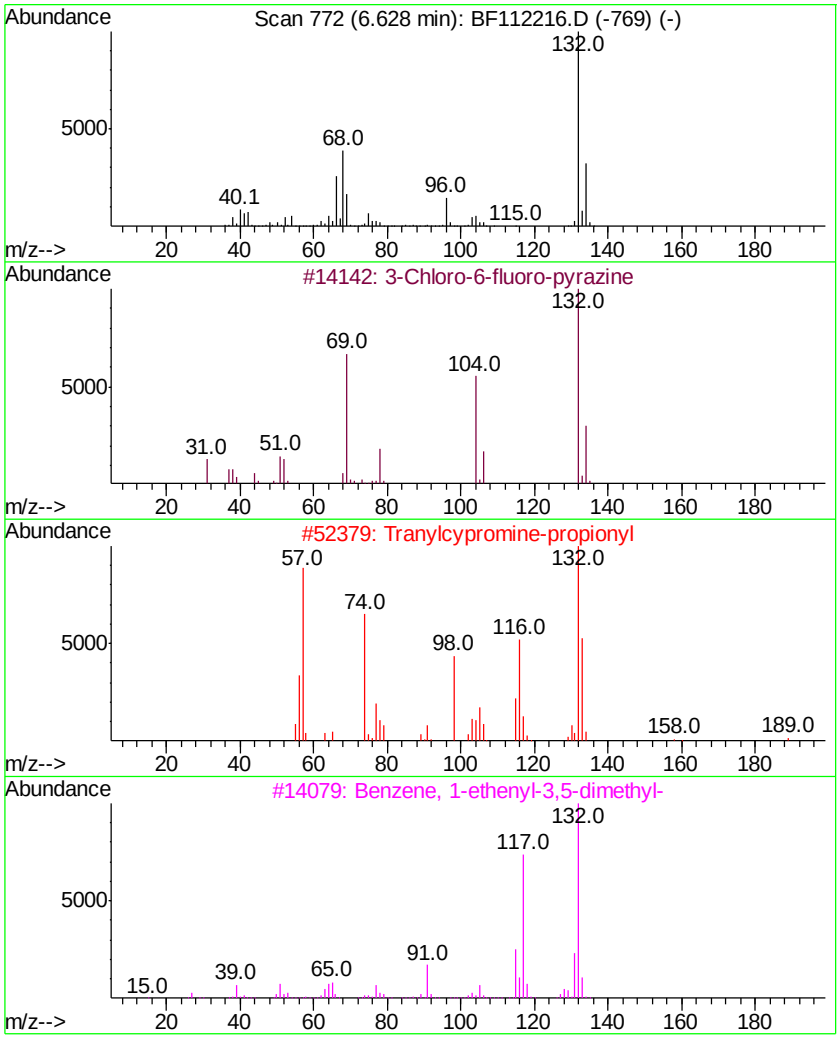
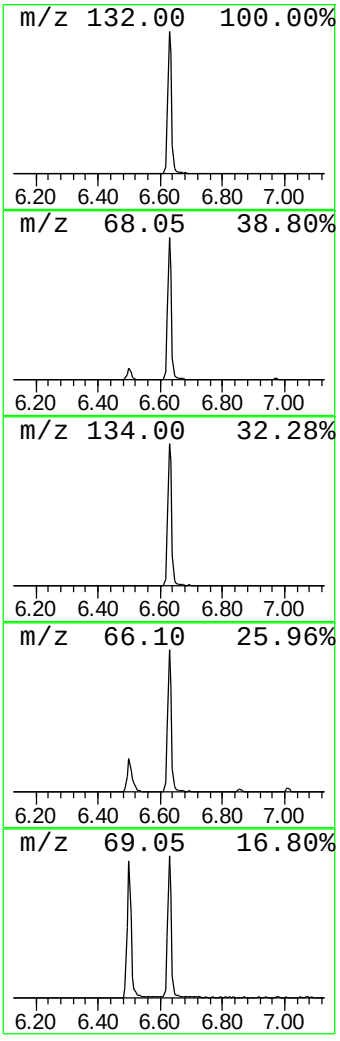
****

Peak Number 1 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	35.84 ng	1758290	1,4-Dichlorobenzene-d4	6.86

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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





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Data File : BF112216.D
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Sample : K1223-04 2X
Misc :
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Instrument : BNA_F
ClientSampleId : TS-P

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

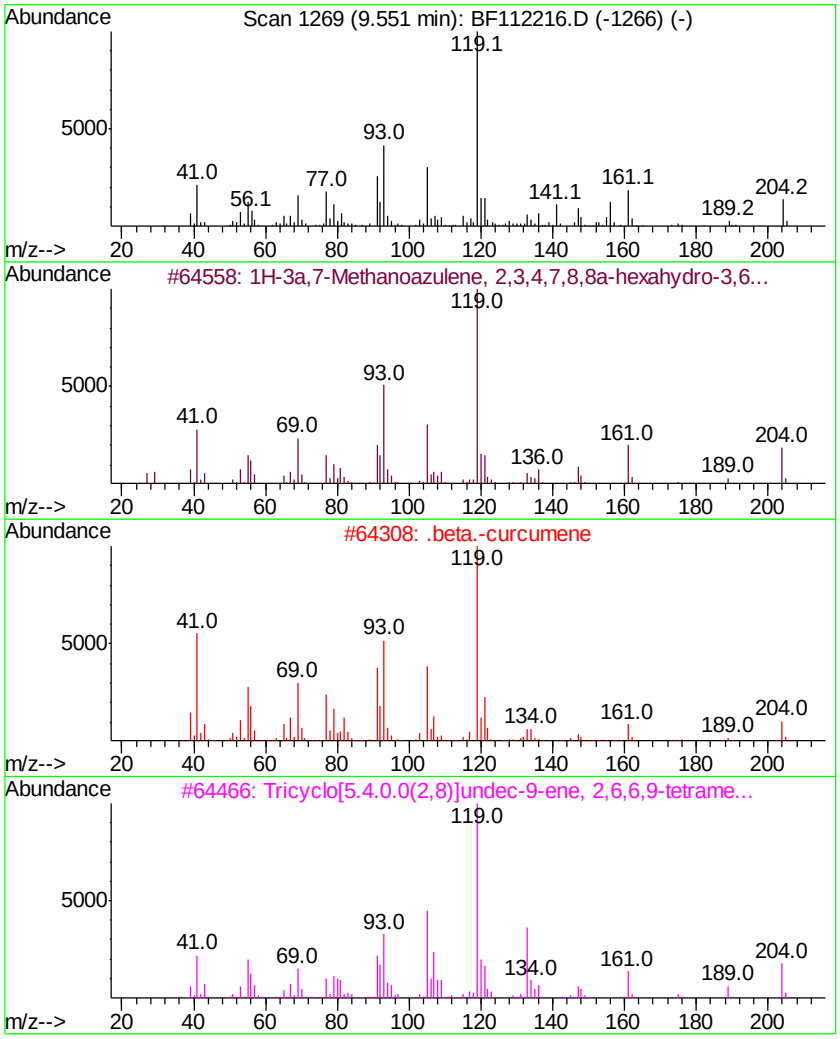
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

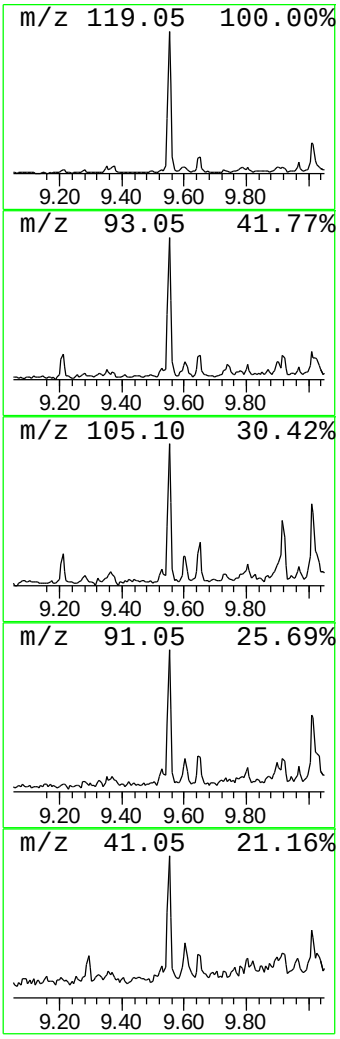
****

Peak Number 3 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	3.54 ng	296721	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	99
2	.beta.-curcumene	204	C15H24	1000374-17-4	83
3	Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	62
4	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	55
5	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	45





Library Search Compound Report

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Instrument : BNA_F
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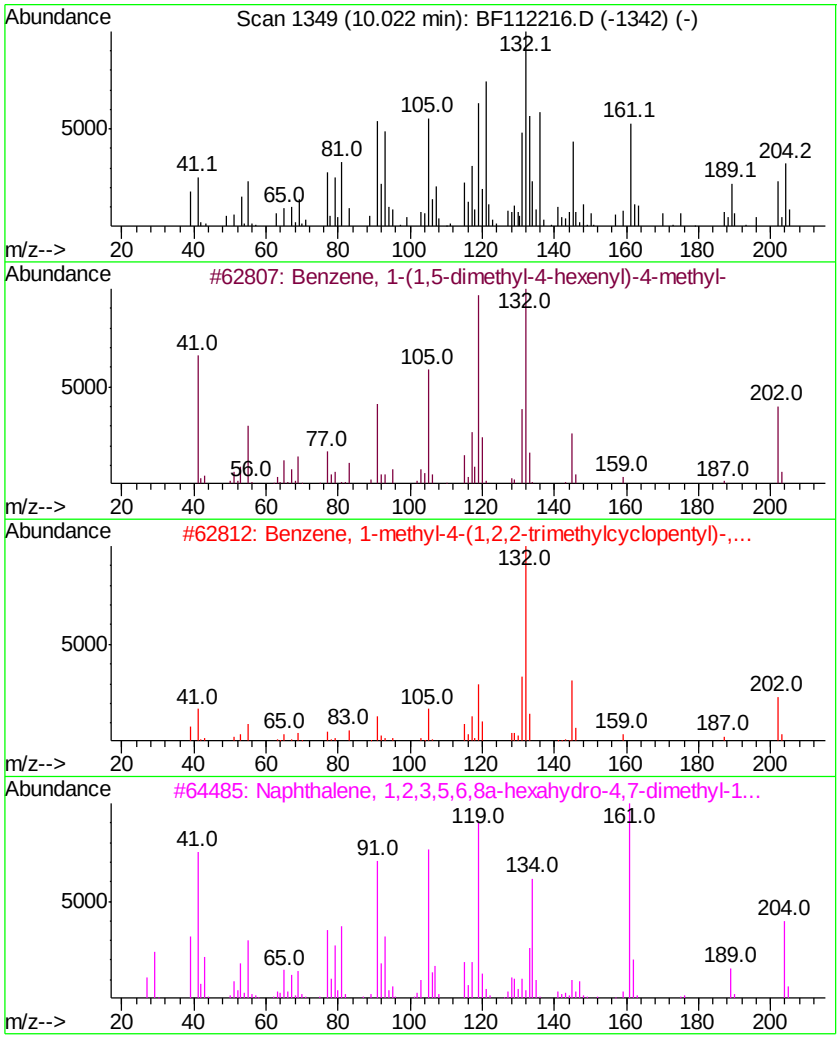
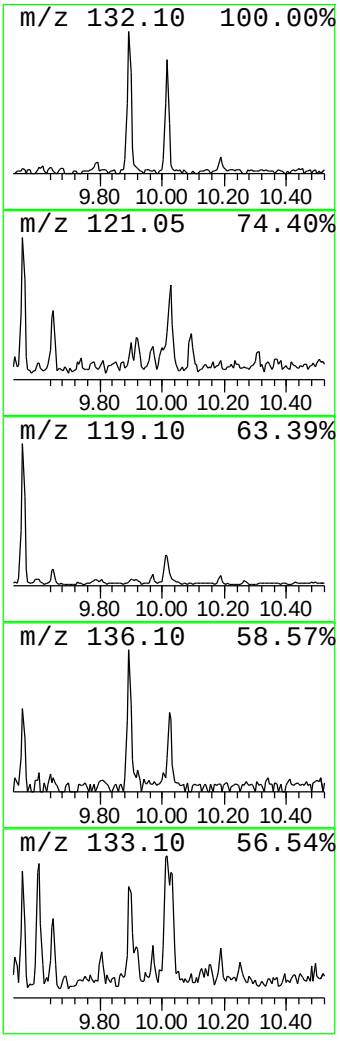
****

Peak Number 4 Benzene, 1-(1,5-dimethyl-4-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	3.23 ng	270529	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(1,5-dimethyl-4-hexen...	202	C15H22	000644-30-4	90
2	Benzene, 1-methyl-4-(1,2,2-trime...	202	C15H22	016982-00-6	89
3	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	89
4	.alpha.-Cubebene	204	C15H24	017699-14-8	52
5	.alfa.-Copaene	204	C15H24	1000360-33-0	52





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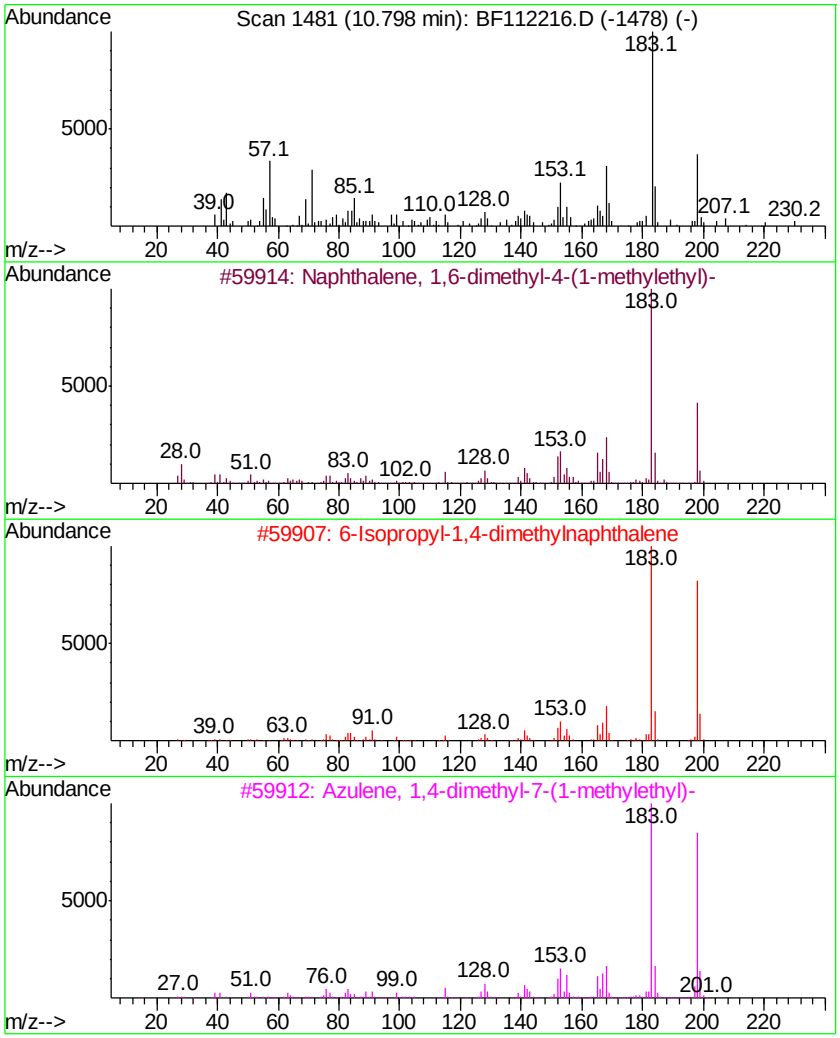
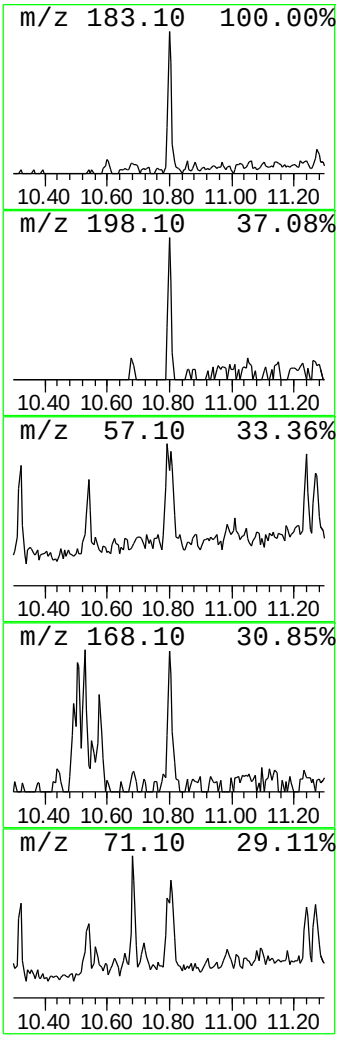
****

Peak Number 5 Naphthalene, 1,6-dimethyl-4... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.16 ng	153681	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	83
2	6-Isopropyl-1,4-dimethylnaphthalene	198	C15H18	000489-77-0	58
3	Azulene, 1,4-dimethyl-7-(1-methy...	198	C15H18	000489-84-9	55
4	2,3-Dihydro-1,3-dimethyl(1H)cycl...	198	C13H14N2	1000112-95-8	47
5	Phenol, 2-(1-phenylethyl)-	198	C14H14O	004237-44-9	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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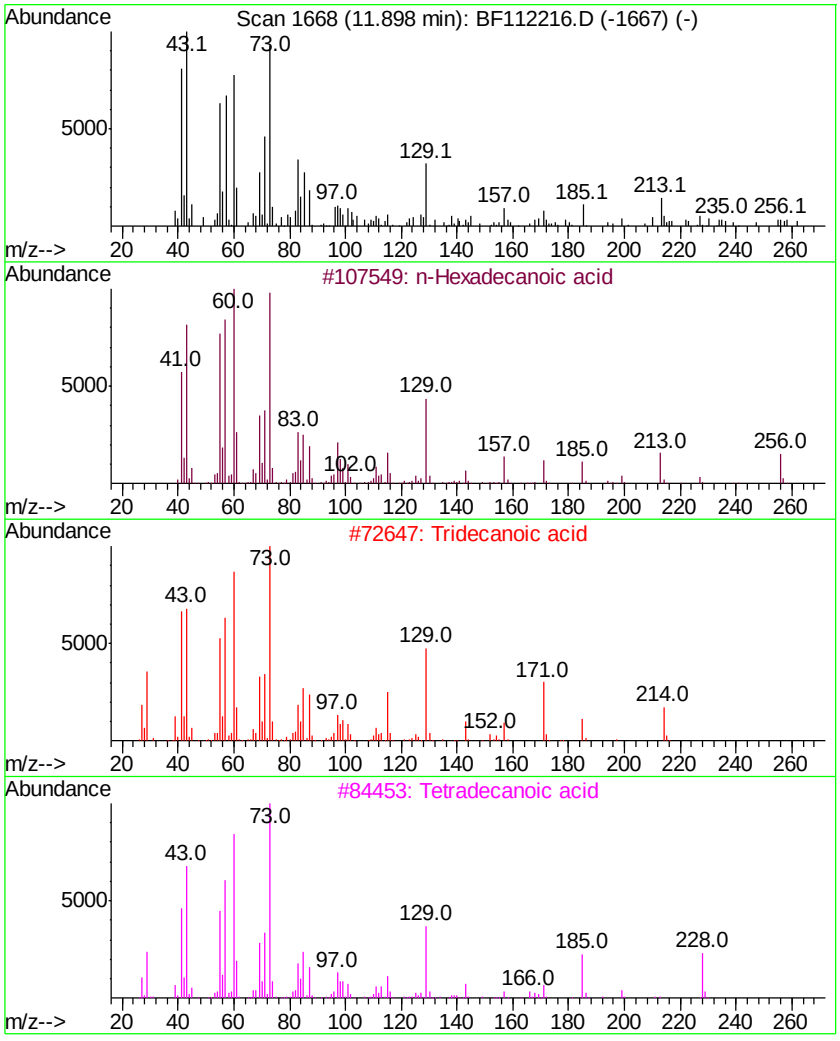
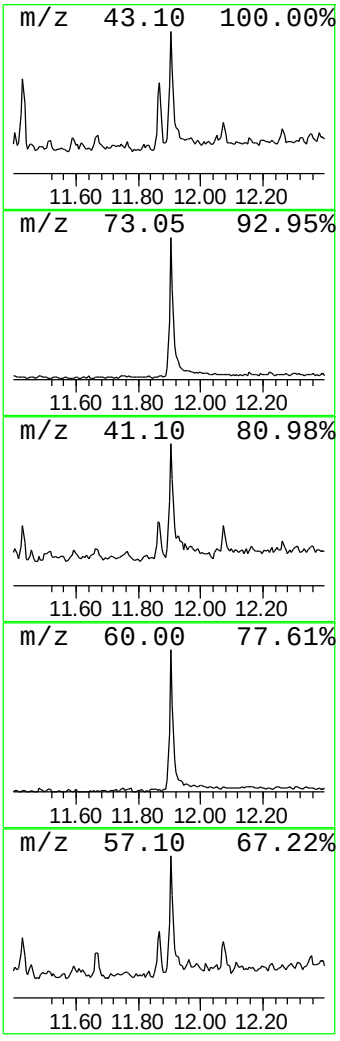
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	5.87 ng	418328	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Octadecanoic acid	284	C18H36O2	000057-11-4	49





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

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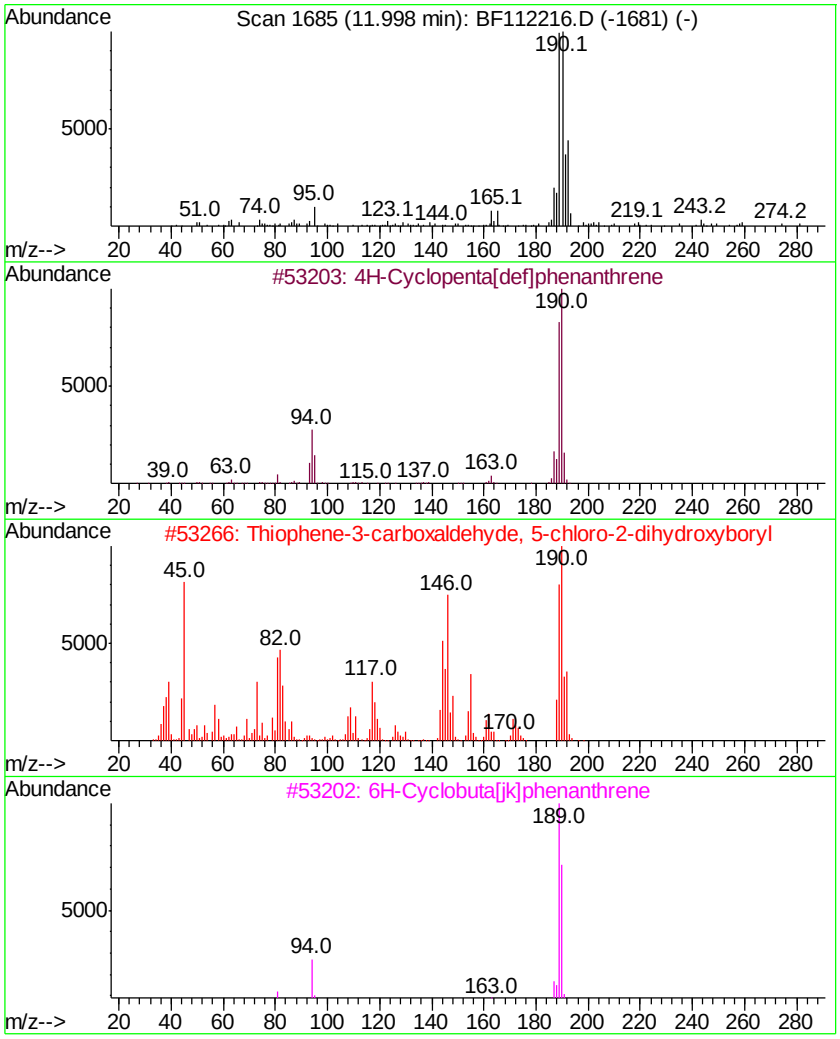
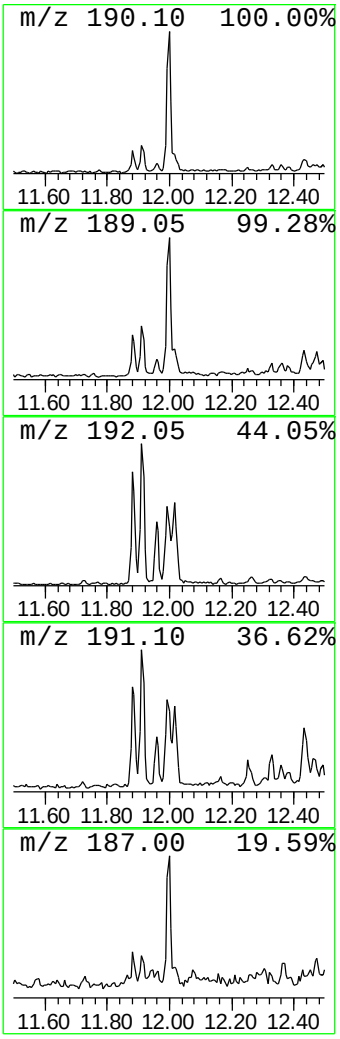
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	2.06 ng	146669	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	68
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38
5	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	33





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-P

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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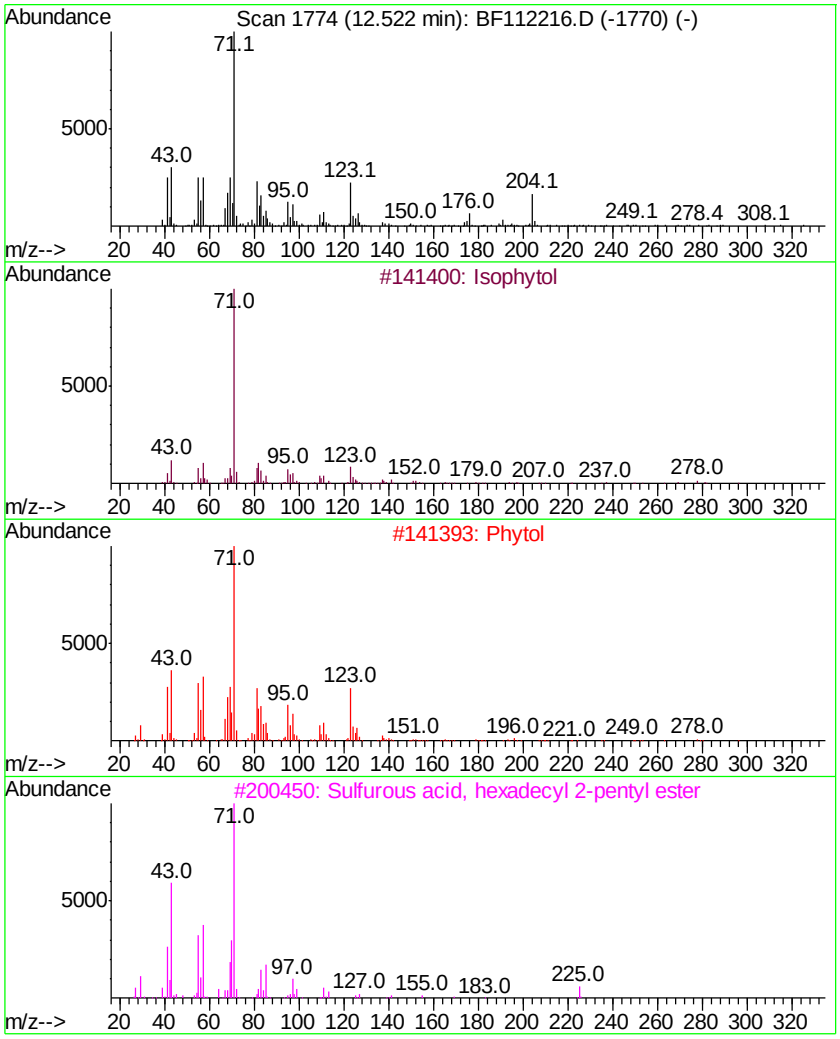
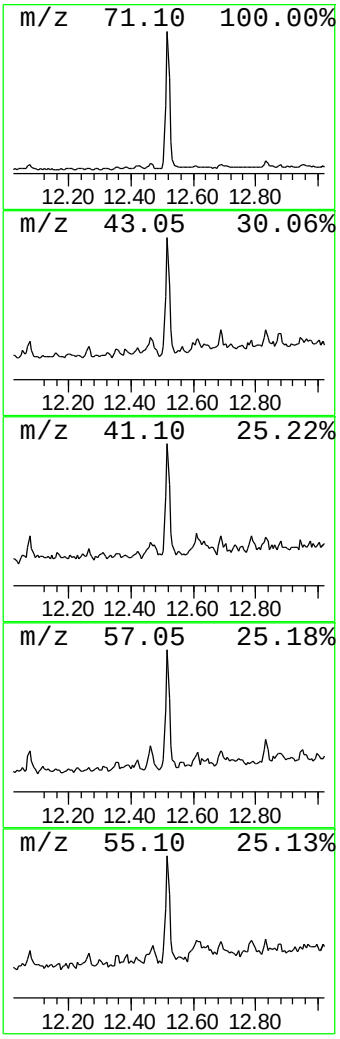
Peak Number 9 Isophytol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	7.04 ng	501870	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophytol	296	C20H40O	000505-32-8	64
2	Phytol	296	C20H40O	000150-86-7	64
3	Sulfurous acid, hexadecyl 2-pent...	376	C21H44O3S	1000309-16-5	52
4	Sulfurous acid, octadecyl 2-pent...	404	C23H48O3S	1000309-16-6	50
5	Butyric acid, 3-pentadecyl ester	298	C19H38O2	1000280-57-3	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112216.D
Acq On : 24 Jan 2019 18:38
Operator : JU/SJ
Sample : K1223-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-P

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

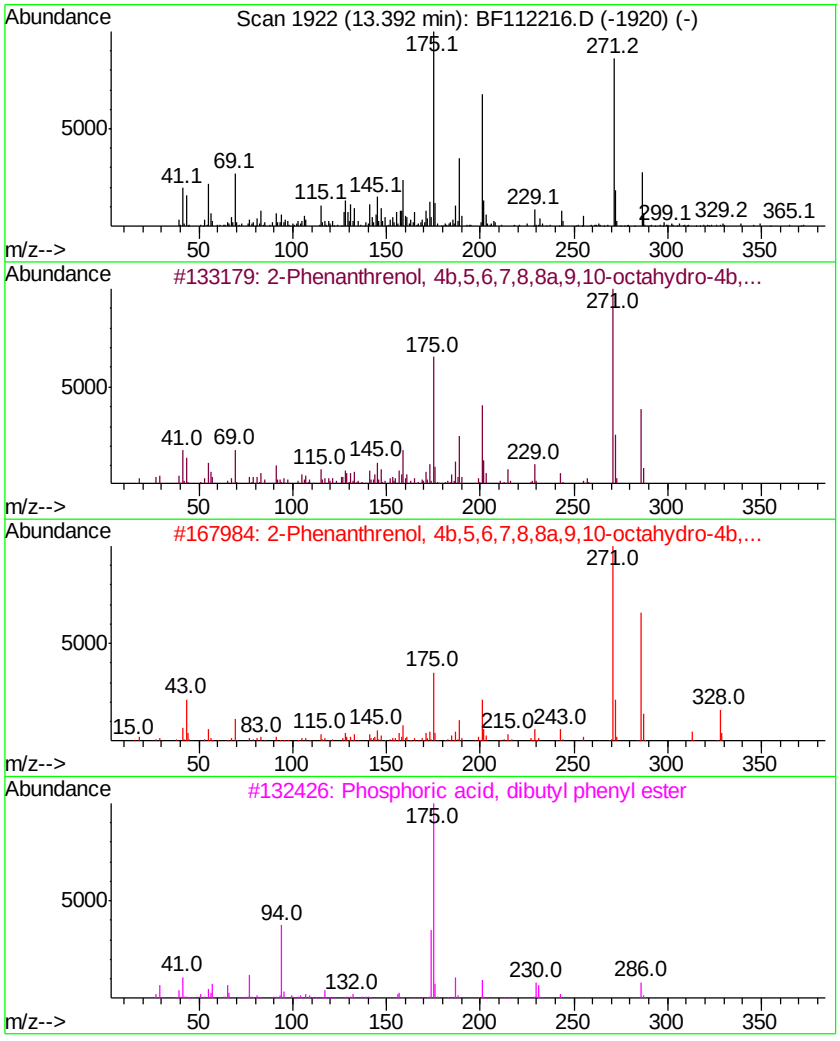
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

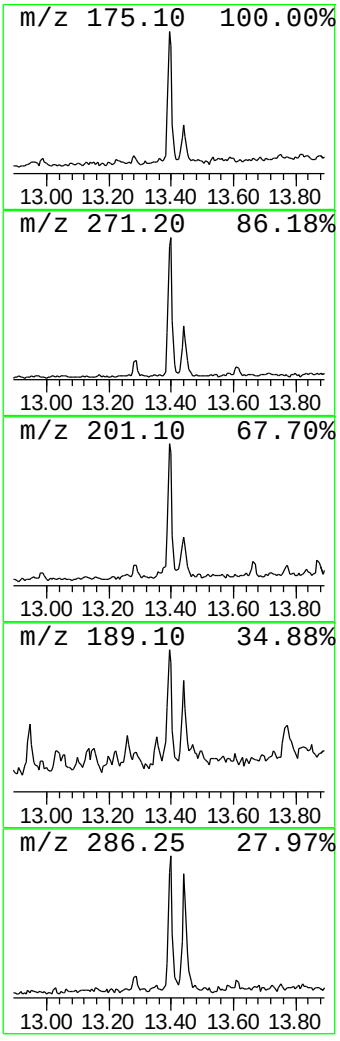
****

Peak Number 10 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	3.56 ng	275359	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	86
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	55
3	Phosphoric acid, dibutyl phenyl ...	286	C14H23O4P	002528-36-1	38
4	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	27
5	4H-Benzo[f]pyrrolo[1,2-a][1,4]di...	354	C22H30N2O2	1000302-50-6	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112216.D
Acq On : 24 Jan 2019 18:38
Operator : JU/SJ
Sample : K1223-04 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-P

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

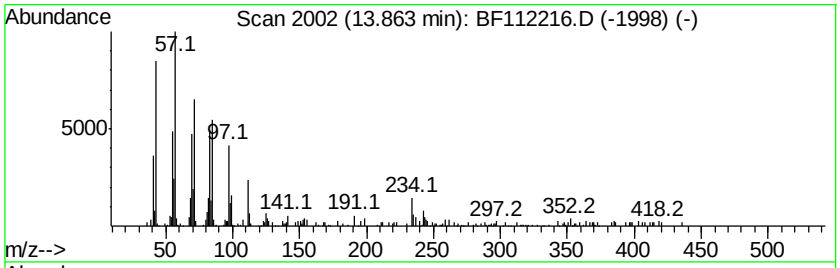
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

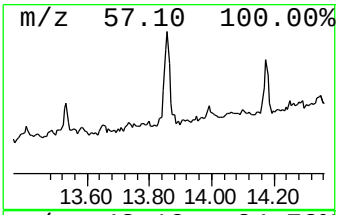
****

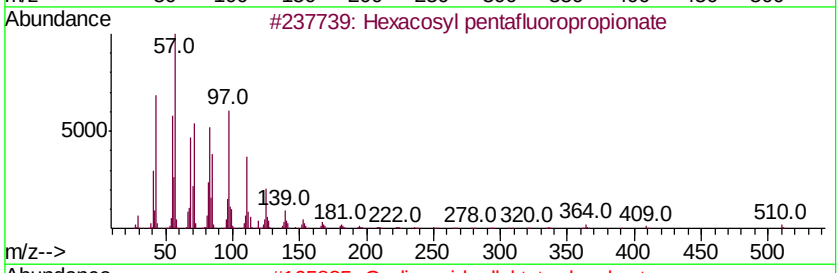
Peak Number 11 Hexacosyl pentafluoropropio... Concentration Rank 5

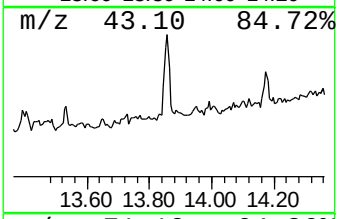
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.06 ng	314711	Chrysene-d12	14.03

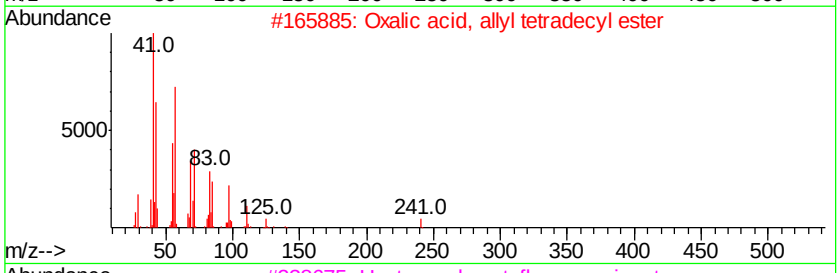
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	83
2	Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	83
3	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	83
4	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	83
5	Cyclooctacosane	392	C28H56	000297-24-5	83

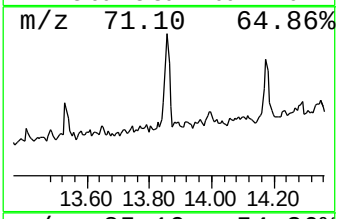


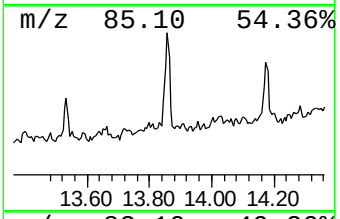


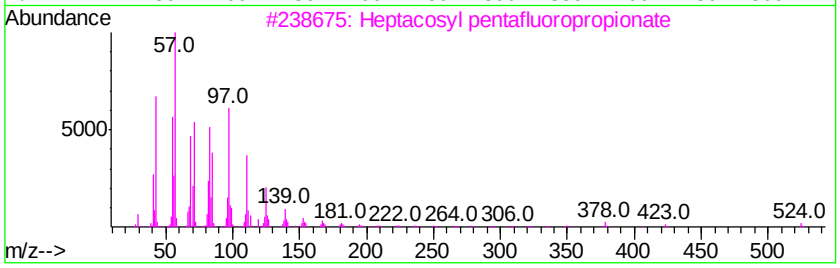


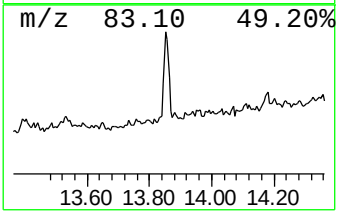












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012419\
Data File : BF112216.D
Acq On : 24 Jan 2019 18:38
Operator : JU/SJ
Sample : K1223-04 2X
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Instrument : BNA_F
ClientSampleId : TS-P

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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
unknown6.63	6.63	35.8	ng	1758290	1	6.86	981311	20.0
1H-3a,7-Methanoaz...	9.55	3.5	ng	296721	3	9.89	1675770	20.0
Benzene, 1-(1,5-d...	10.02	3.2	ng	270529	3	9.89	1675770	20.0
Naphthalene, 1,6-...	10.80	2.2	ng	153681	4	11.38	1425170	20.0
n-Hexadecanoic acid	11.90	5.9	ng	418328	4	11.38	1425170	20.0
4H-Cyclopenta[def...	12.00	2.1	ng	146669	4	11.38	1425170	20.0
Isophytol	12.52	7.0	ng	501870	4	11.38	1425170	20.0
2-Phenanthrenol, ...	13.39	3.6	ng	275359	5	14.03	1548920	20.0
Hexacosyl pentafl...	13.86	4.1	ng	314711	5	14.03	1548920	20.0