LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

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-BF110818.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	2.140	6	9	17	rVV	45488	68997	3.40%	0.182%
2	5.534	583	586	592	rBV	53309	75316	3.71%	0.199%
3	6.763	792	795	802	rVB	116635	105631	5.20%	0.279%
4	6.945	823	826	832	rBV	497852	446591	21.99%	1.180%
5	7.098	849	852	860	rBV3	65908	73835	3.64%	0.195%
6	7.245	874	877	885	rVB2	59959	78221	3.85%	0.207%
7	7.451	909	912	914	rBV	73426	60288	2.97%	0.159%
8	8.010	1004	1007	1012	rVB	59790	65252	3.21%	0.172%
9	8.228	1040	1044	1046	rBV	613372	548722	27.02%	1.450%
10	8.245	1046	1047	1051	rVV3	77980	80039	3.94%	0.212%
11	8.298	1051	1056	1059	rVB3	48769	69973	3.45%	0.185%
12	8.586	1101	1105	1108	rBV2	52103	63920	3.15%	0.169%
13	8.722	1125	1128	1130	rBV	282625	217257	10.70%	0.574%
14	8.775	1133	1137	1139	rBV3	47903	60101	2.96%	0.159%
15	8.881	1151	1155	1160	rBV2	117574	157534	7.76%	0.416%
16	8.922	1160	1162	1164	rBV2	49541	52810	2.60%	0.140%
17	8.963	1167	1169	1174	rVB2	89374	96701	4.76%	0.256%
18	9.004	1174	1176	1178	rBV	49114	53006	2.61%	0.140%
19	9.028	1178	1180	1181	rBV	76907	52895	2.60%	0.140%
20	9.057	1181	1185	1189	rVB4	61865	98634	4.86%	0.261%
21	9.145	1194	1200	1204	rBV	223636	402869	19.84%	1.065%
22	9.181	1204	1206	1210	rVB	275876	256786	12.64%	0.679%
23	9.222	1210	1213	1216	rBV2	197729	233016	11.47%	0.616%
24	9.251	1216	1218	1222	rVB2	158107	156146	7.69%	0.413%
25	9.298	1222	1226	1229	rBV4	166464	246175	12.12%	0.651%
26	9.328	1229	1231	1233	rVV2	86566	61481	3.03%	0.162%
27	9.357	1233	1236	1240	rBV	685445	582595	28.69%	1.540%
28	9.433	1247	1249	1253	rBV	147738	153346	7.55%	0.405%
29	9.481	1253	1257	1260	rVB3	637939	748149	36.84%	1.977%
30	9.528	1263	1265	1268	rBV	195824	175089	8.62%	0.463%
31	9.551	1268	1269	1271	rVV	117226	75726	3.73%	0.200%
32	9.575	1271	1273	1275	rVV	74006	60355	2.97%	0.160%
33	9.598	1275	1277	1282	rVB2	86119	79026	3.89%	0.209%
34	9.639	1282	1284	1289	rVB4	68749	79026	3.89%	0.209%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

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-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.686	1289	1292	1294	rBV	111107	84670	4.17%	0.224%
36	9.716	1294	1297	1303	rVB4	143289	205796	10.13%	0.544%
37	9.775	1303	1307	1308	rBV3	66996	88634	4.36%	0.234%
38	9.857	1319	1321	1325	rVB	76772	84268	4.15%	0.223%
39	9.892	1325	1327	1331	rBV4	52889	57595	2.84%	0.152%
40	9.933	1331	1334	1338	rBV	259488	308706	15.20%	0.816%
41	9.986	1338	1343	1346	rBV2	671062	687930	33.87%	1.818%
42	10.039	1350	1352	1355	rVV	221574	167803	8.26%	0.443%
43	10.157	1370	1372	1373	rVV	71540	53607	2.64%	0.142%
44	10.175	1373	1375	1377	rVB	86342	62625	3.08%	0.166%
45	10.239	1383	1386	1387	rBV	58967	63359	3.12%	0.167%
46	10.339	1400	1403	1404	rBV	83119	76617	3.77%	0.202%
47	10.357	1404	1406	1408	rVB2	86718	68936	3.39%	0.182%
48	10.386	1408	1411	1412	rBV2	116437	123590	6.09%	0.327%
49	10.445	1418	1421	1424	rBV	423389	350577	17.26%	0.927%
50	10.498	1428	1430	1432	rBV	227111	219132	10.79%	0.579%
51	10.616	1448	1450	1453	rVB	211265	191107	9.41%	0.505%
52	10.786	1477	1479	1482	rVB	211691	179258	8.83%	0.474%
53	10.851	1486	1490	1492	rBV	493026	628694	30.96%	1.662%
54	10.969	1506	1510	1517	rBV3	339519	676088	33.29%	1.787%
55	11.027	1517	1520	1522	rVB	1383935	1120632	55.18%	2.962%
56	11.110	1531	1534	1538	rVB	743739	614241	30.25%	1.623%
57	11.145	1538	1540	1543	rVB	230503	205445	10.12%	0.543%
58	11.180	1543	1546	1550	rVB2	217439	253238	12.47%	0.669%
59	11.222	1551	1553	1555	rBV	96621	66824	3.29%	0.177%
60	11.351	1573	1575	1579	rBV3	95131	120760	5.95%	0.319%
61	11.404	1581	1584	1587	rVB	319947	271852	13.39%	0.718%
62	11.463	1591	1594	1595	rBV	144654	136908	6.74%	0.362%
63	11.480	1595	1597	1598	rBV	455736	354036	17.43%	0.936%
64	11.498	1598	1600	1603	rVB2	550466	482385	23.75%	1.275%
65	11.539	1604	1607	1608	rBV2	169306	166675	8.21%	0.441%
66	11.669	1627	1629	1632	rVB	261110	228961	11.27%	0.605%
67	11.845	1656	1659	1662	rBV	934337	740250	36.45%	1.956%
68	11.874	1662	1664	1668	rVV2	229992	298135	14.68%	0.788%
69	11.916	1668	1671	1675	rVB	659617	637376	31.38%	1.685%
70	11.980	1680	1682	1685	rVV	185607	176281	8.68%	0.466%
71	12.098	1699	1702	1705	rVB	329218	290815	14.32%	0.769%

LSC Area Percent Report

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Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

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-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.269	1728	1731	1735	rVB2	954483	1338094	65.89%	3.537%
73	12.433	1756	1759	1764	rVB	1460998	1391376	68.51%	3.677%
74	12.492	1766	1769	1773	rVB	527274	558475	27.50%	1.476%
75	12.833	1825	1827	1832	rBV	499152	494893	24.37%	1.308%
76	13.186	1884	1887	1890	rBV	533401	516923	25.45%	1.366%
77	13.516	1940	1943	1947	rVB	870394	811178	39.94%	2.144%
78	13.657	1964	1967	1970	rBV	1476109	1463114	72.04%	3.867%
79	13.692	1970	1973	1975	rVV	454000	356199	17.54%	0.941%
80	14.010	2024	2027	2031	rVB	630209	700910	34.51%	1.852%
81	14.051	2031	2034	2036	rBV	356397	335633	16.53%	0.887%
82	14.139	2046	2049	2053	rVB2	752010	913988	45.01%	2.416%
83	14.268	2069	2071	2075	rVB2	376216	396469	19.52%	1.048%
84	14.310	2075	2078	2083	rBV3	566307	898794	44.26%	2.375%
85	14.445	2098	2101	2105	rVB2	488895	491029	24.18%	1.298%
86	14.498	2107	2110	2114	rBV4	315570	475233	23.40%	1.256%
87	14.568	2119	2122	2126	rVB2	260753	289508	14.26%	0.765%
88	14.610	2126	2129	2134	rBV	1000070	1182817	58.24%	3.126%
89	14.751	2149	2153	2159	rVB2	1619622	2030851	100.00%	5.367%
90	14.804	2159	2162	2167	rVB3	415351	611630	30.12%	1.617%
91	15.104	2209	2213	2216	rVV	417019	459287	22.62%	1.214%
92	15.145	2217	2220	2226	rVB3	227473	400086	19.70%	1.057%
93	15.457	2270	2273	2278	rVB	307320	400624	19.73%	1.059%
94	15.668	2306	2309	2313	rVB	169201	177736	8.75%	0.470%
95	15.880	2340	2345	2349	rVB	479686	694928	34.22%	1.837%
96	16.092	2376	2381	2389	rVB2	905007	1639055	80.71%	4.332%
97	16.627	2468	2472	2482	rVB	199697	352048	17.33%	0.930%
98	17.186	2563	2567	2573	rVB	123024	216883	10.68%	0.573%
99	17.898	2681	2688	2696	rVB	224257	539199	26.55%	1.425%
100	18.262	2742	2750	2761	rVB2	479375	1320306	65.01%	3.489%

Sum of corrected areas: 37836580

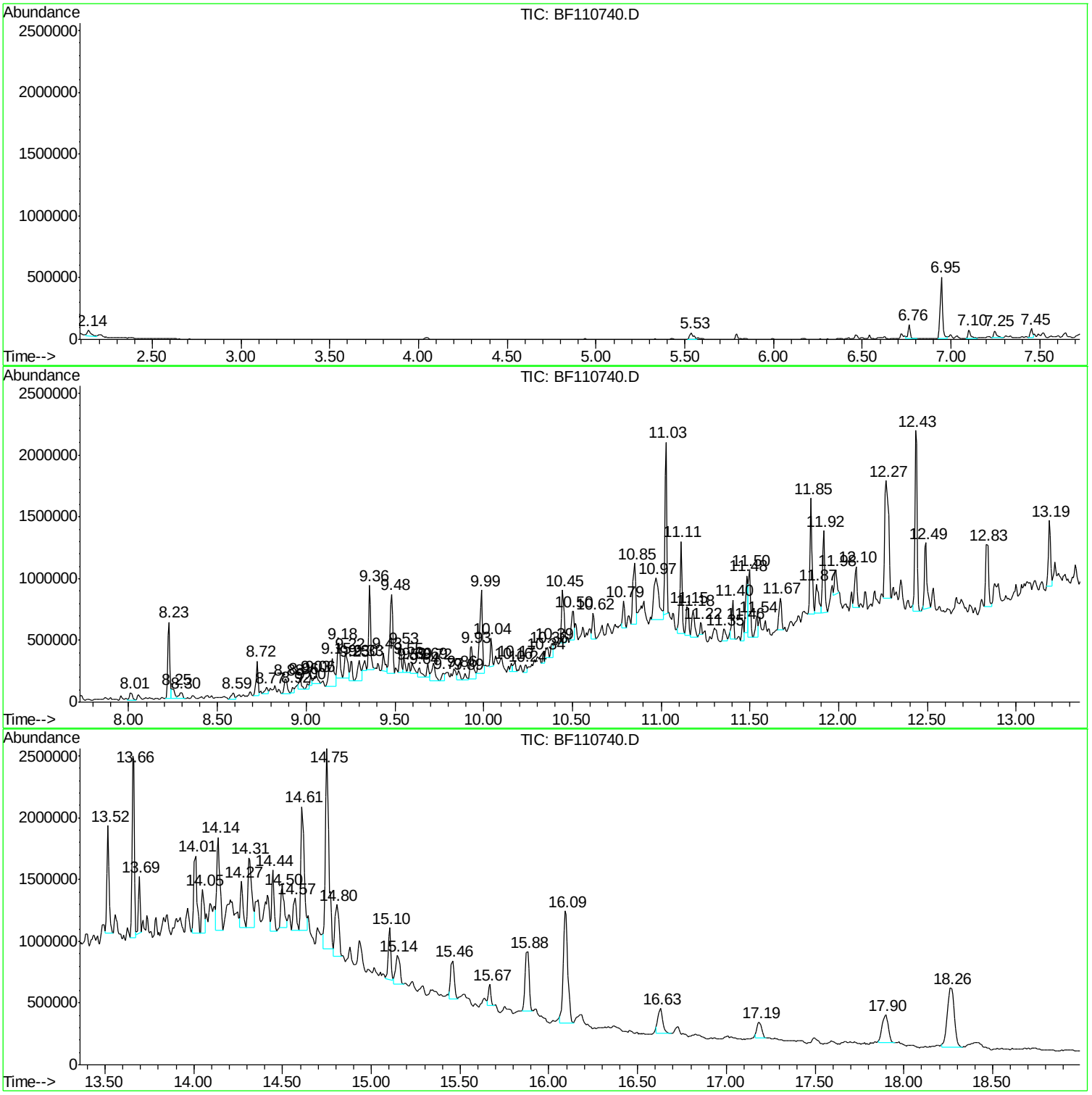
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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 F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

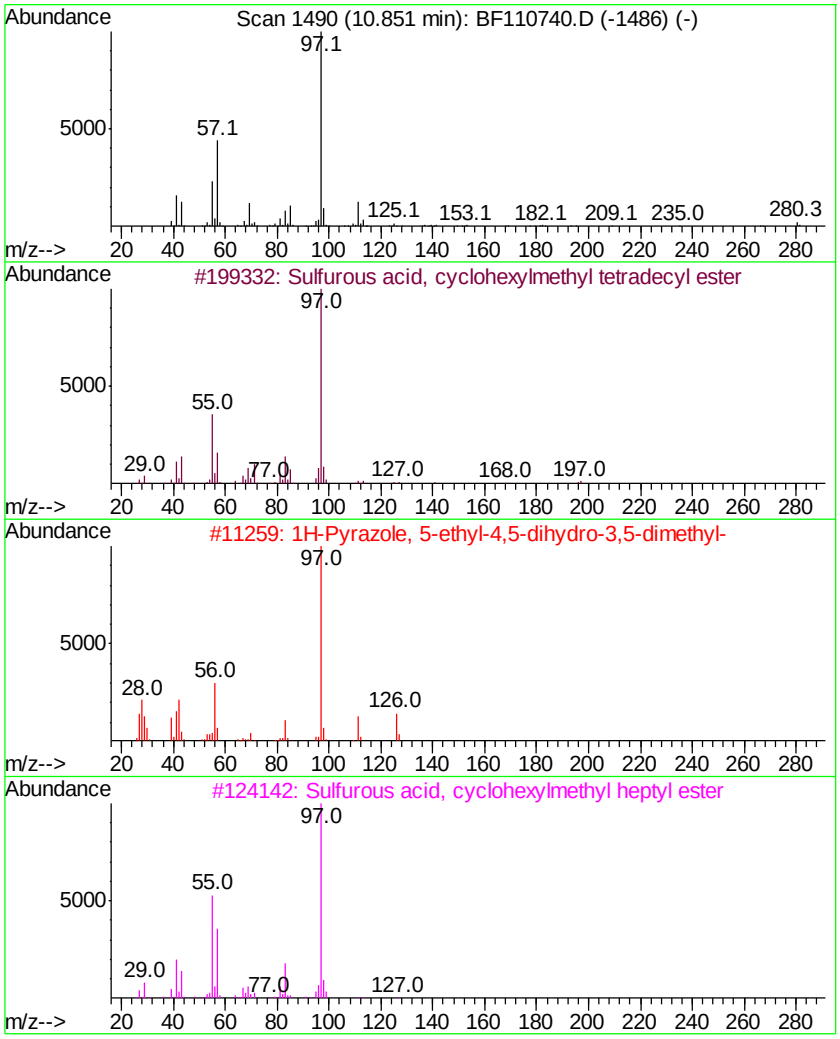
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

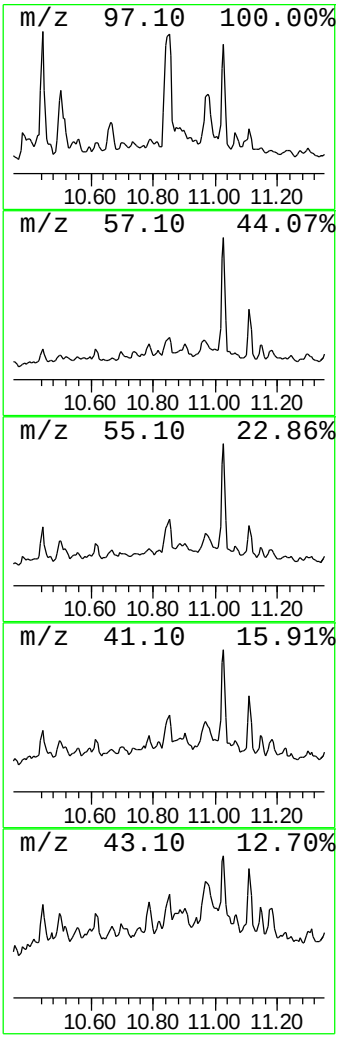
****

Peak Number 1 Sulfurous acid, cyclohexylm... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	35.52 ng	628694	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	56
2	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	53
3	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	53
4	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	53
5	2-Ethoxy-4-methyl-pent-2-enoic acid	158	C8H14O3	1000190-08-8	50





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

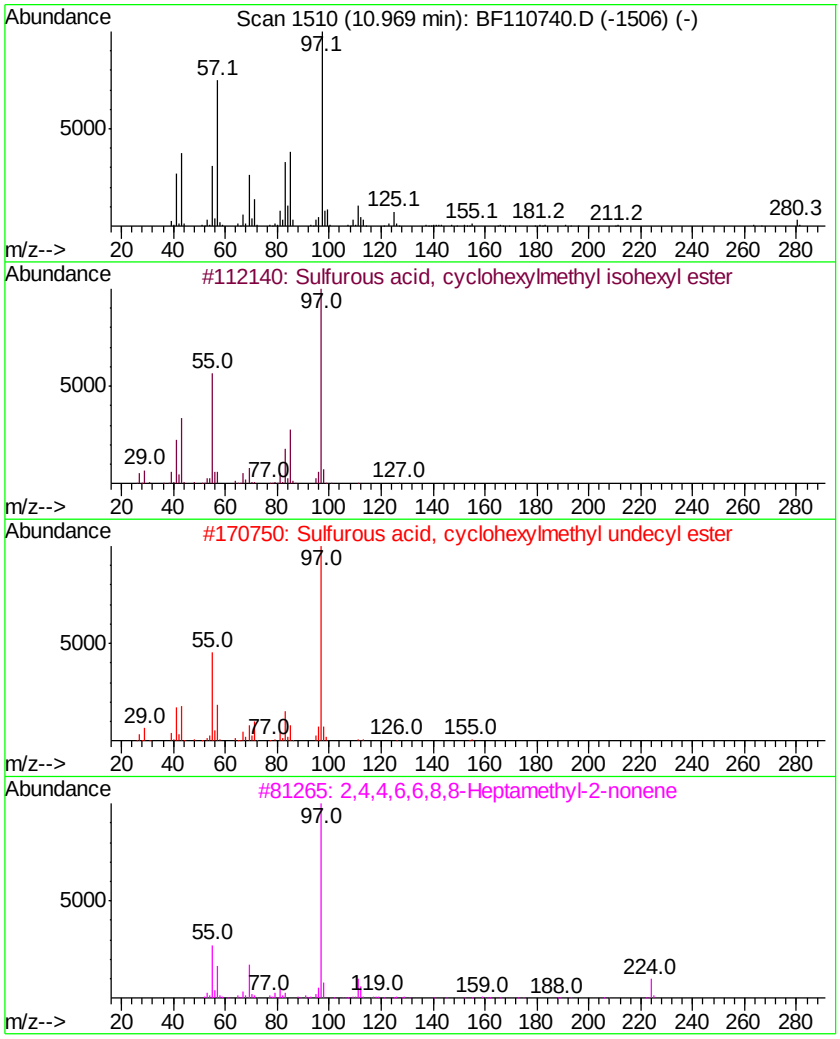
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

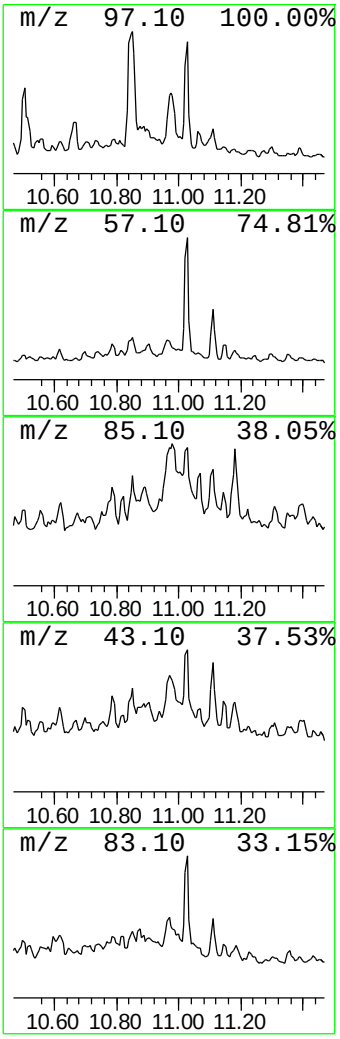
****

Peak Number 2 Sulfurous acid, cyclohexylm... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	38.19 ng	676088	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	59
2	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	43
3	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	38
4	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	27
5	Bicyclo[3.2.0]heptan-2-one, 6-hy...	166	C10H14O2	1000154-96-8	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
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Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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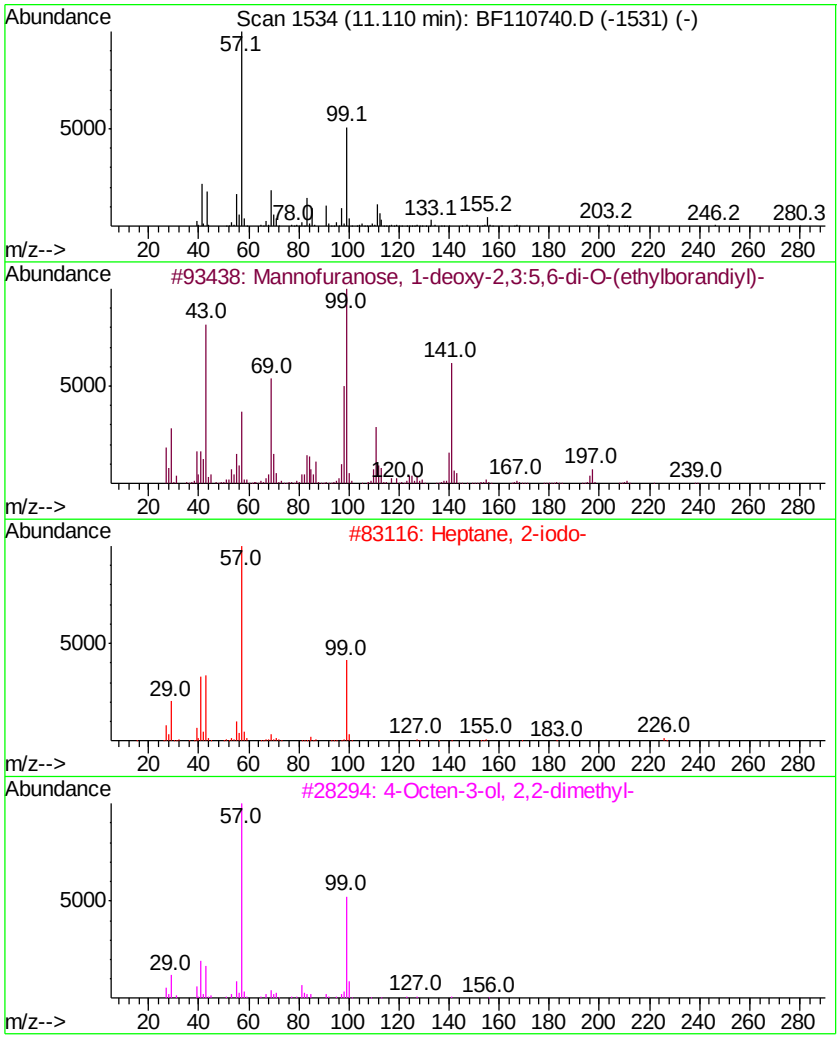
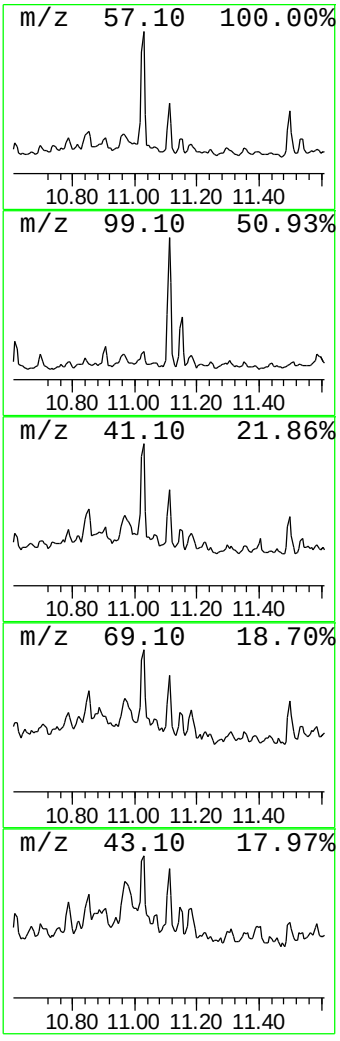
Peak Number 4 unknown11.11 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.11	34.70 ng	614241	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mannofuranose, 1-deoxy-2,3:5,6-d...	240	C10H18B2O5	1000150-85-3	37
2	Heptane, 2-iodo-	226	C7H15I	018589-29-2	32
3	4-Octen-3-ol, 2,2-dimethyl-	156	C10H20O	053960-44-4	32
4	2-Propylthiazole	127	C6H9NS	017626-75-4	30
5	2-Azido-2,4,4,6,6,8,8-heptamethy...	267	C16H33N3	1000293-29-1	27





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Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
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Misc :
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Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

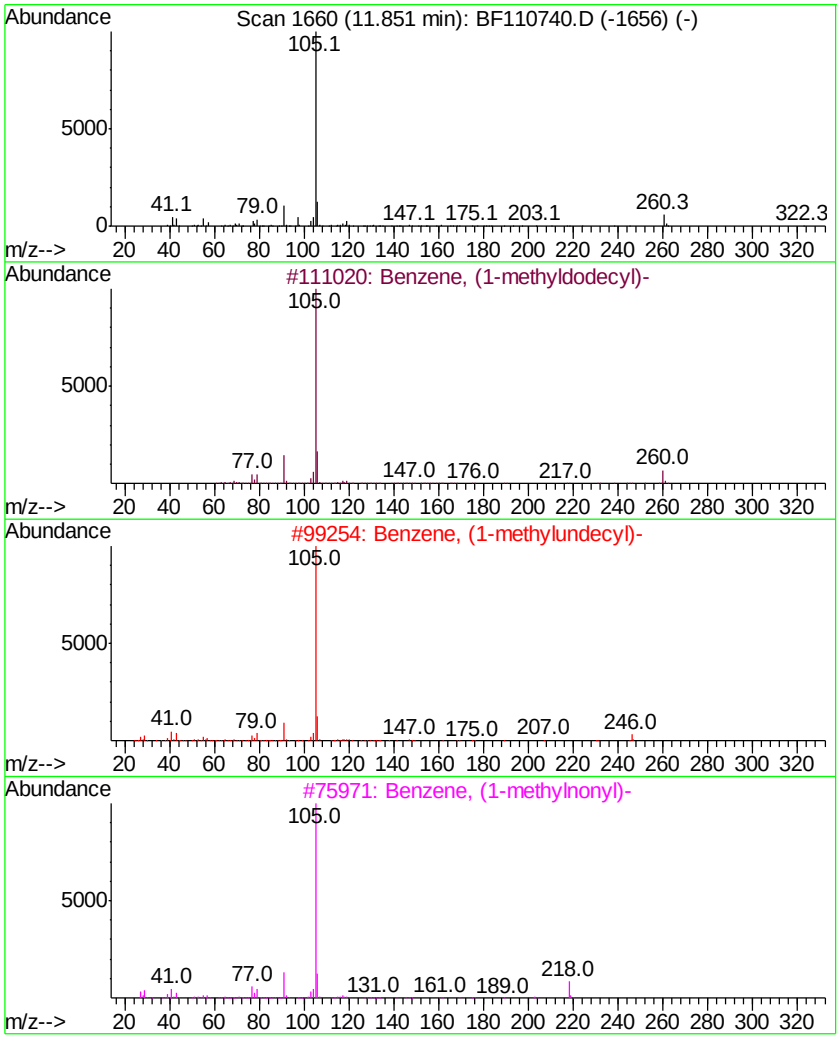
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

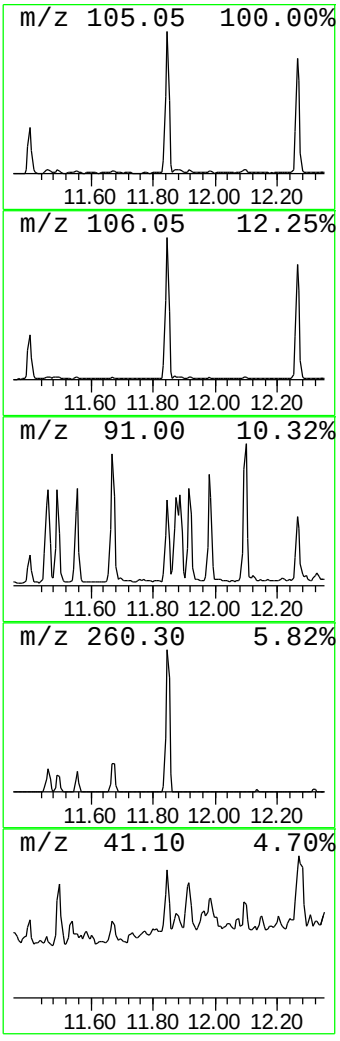
****

Peak Number 5 Benzene, (1-methyldodecyl)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	41.82 ng	740250	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	93
2	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
3	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	64
4	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	64
5	1-Hexene, 3-methyl-6-phenyl-4-(1...	294	C21H26O	1000194-52-4	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

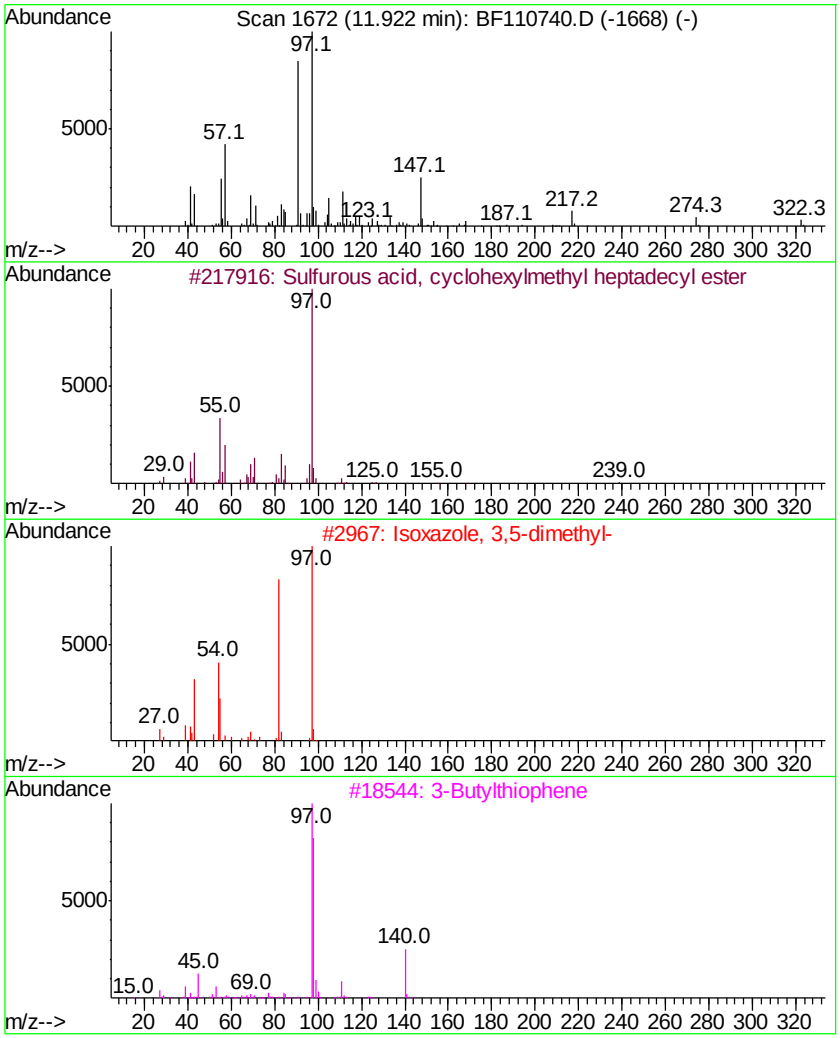
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

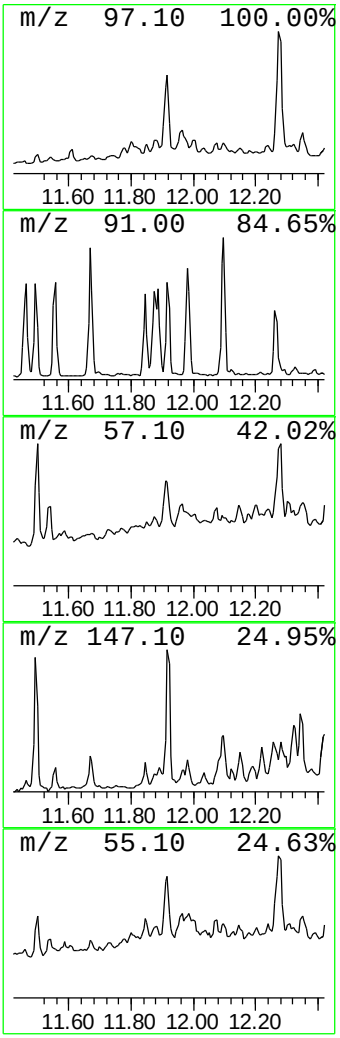
****

Peak Number 6 Sulfurous acid, cyclohexylm... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	36.01 ng	637376	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	64
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
3	3-Butylthiophene	140	C8H12S	034722-01-5	53
4	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	53
5	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	50





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Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

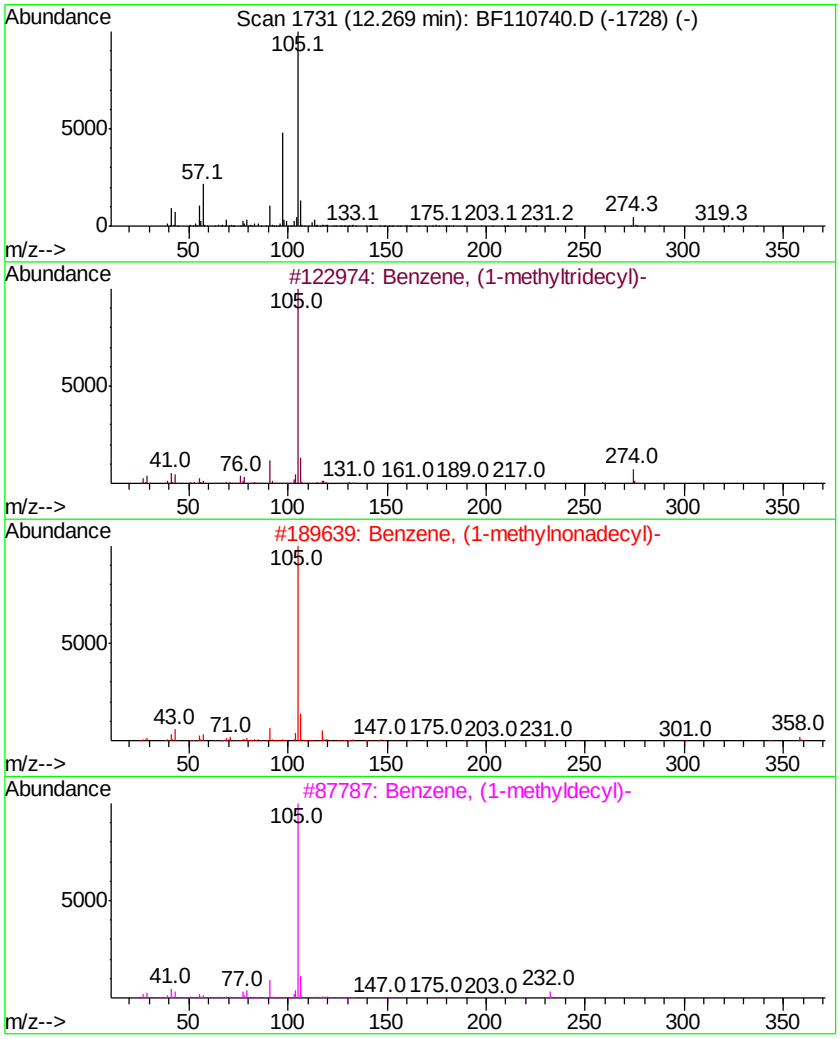
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

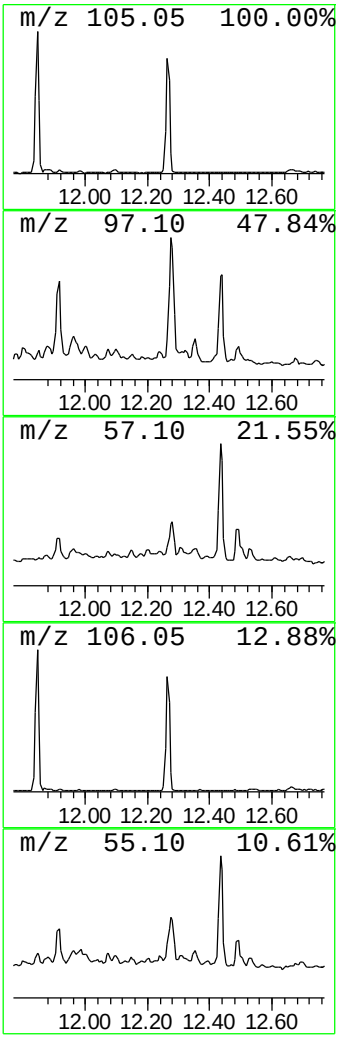
****

Peak Number 7 unknown12.27 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	75.59 ng	1338090	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	43
2	Benzene, (1-methylnonadecyl)-	358	C26H46	002398-66-5	27
3	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	27
4	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	27
5	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	22





Library Search Compound Report

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Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

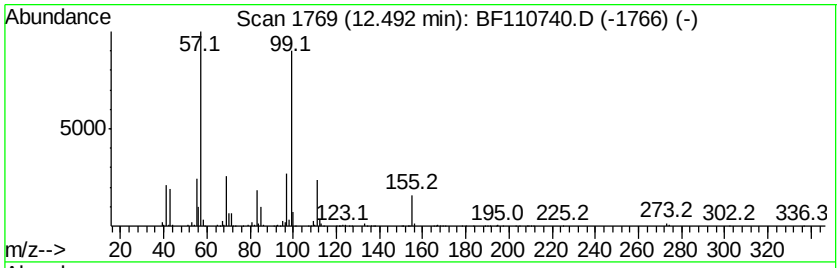
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

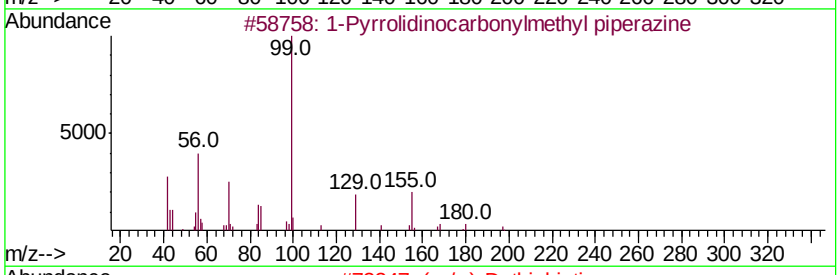
****

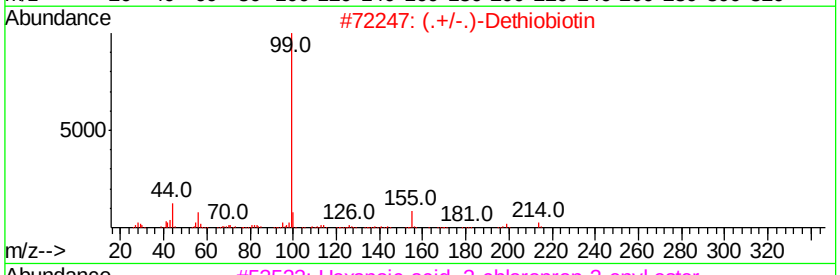
Peak Number 9 unknown12.49 Concentration Rank 19

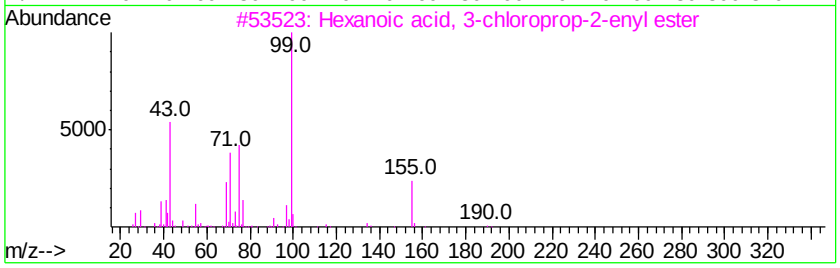
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	31.55 ng	558475	Phenanthrene-d10	11.48

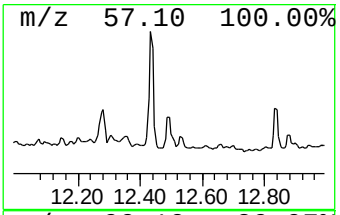
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	47
2	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	43
3	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	37
4	Ethyl .alpha.-bromocyclobutaneca...	206	C7H11BrO2	035120-18-4	35
5	2-Propylthiazole	127	C6H9NS	017626-75-4	35

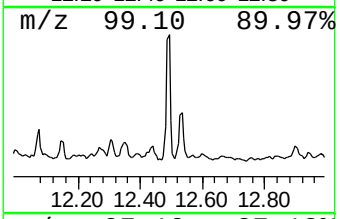


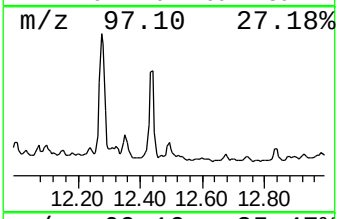


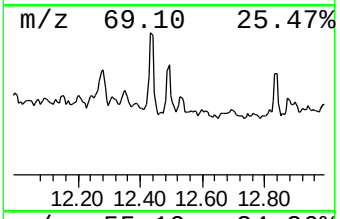


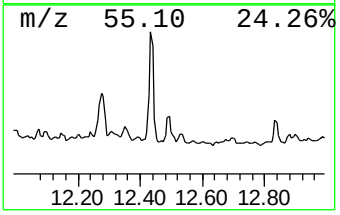












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Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

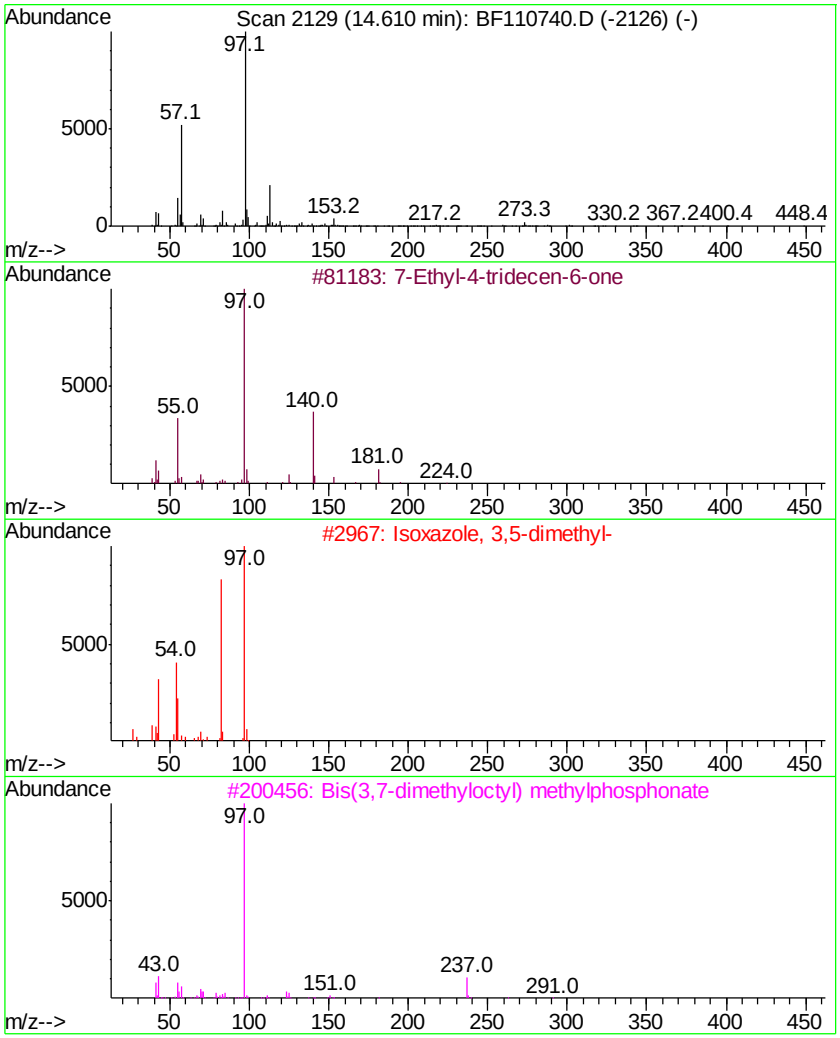
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

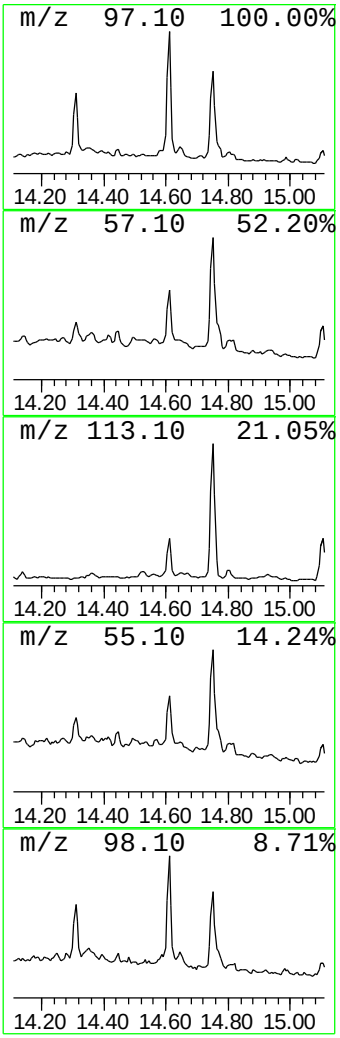
****

Peak Number 11 7-Ethyl-4-tridecen-6-one Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	25.88 ng	1182820	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Ethyl-4-tridecen-6-one	224	C15H28O	1000374-07-1	53
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	50
3	Bis(3,7-dimethyloctyl) methylpho...	376	C21H45O3P	1000298-35-2	50
4	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	47
5	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	42





Library Search Compound Report

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Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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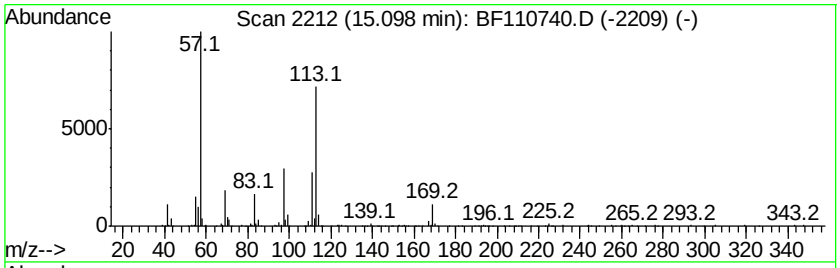
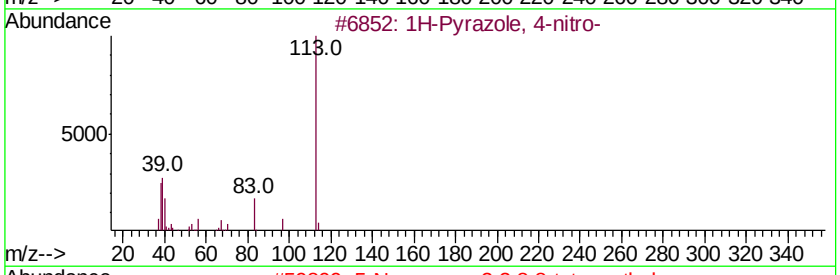
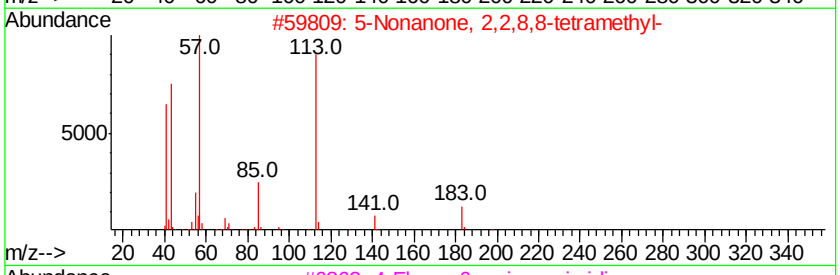
Peak Number 13 unknown15.10 Concentration Rank 8

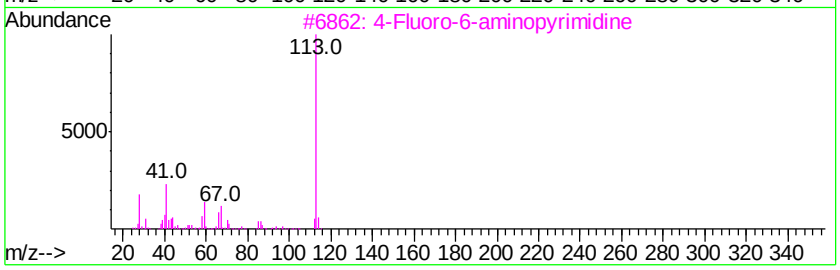
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	51.68 ng	459287	Perylene-d12	15.67

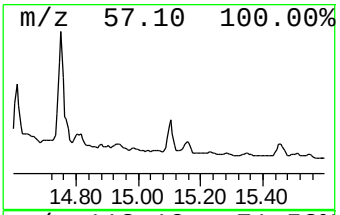
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 4-nitro-	113	C3H3N3O2	002075-46-9	43
2	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	38
3	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	38
4	Boronic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	38
5	2,5-Pyrrolidinedione, 3-methyl-4...	155	C8H13NO2	016493-22-4	38

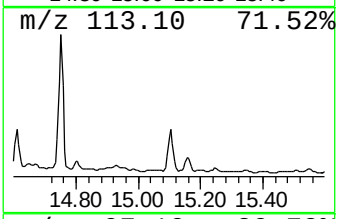


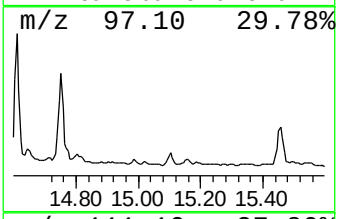


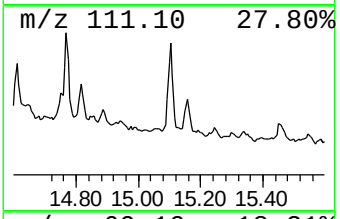


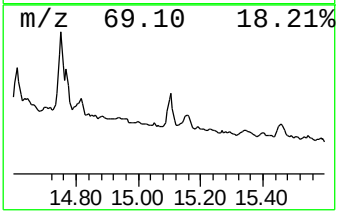












Library Search Compound Report

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Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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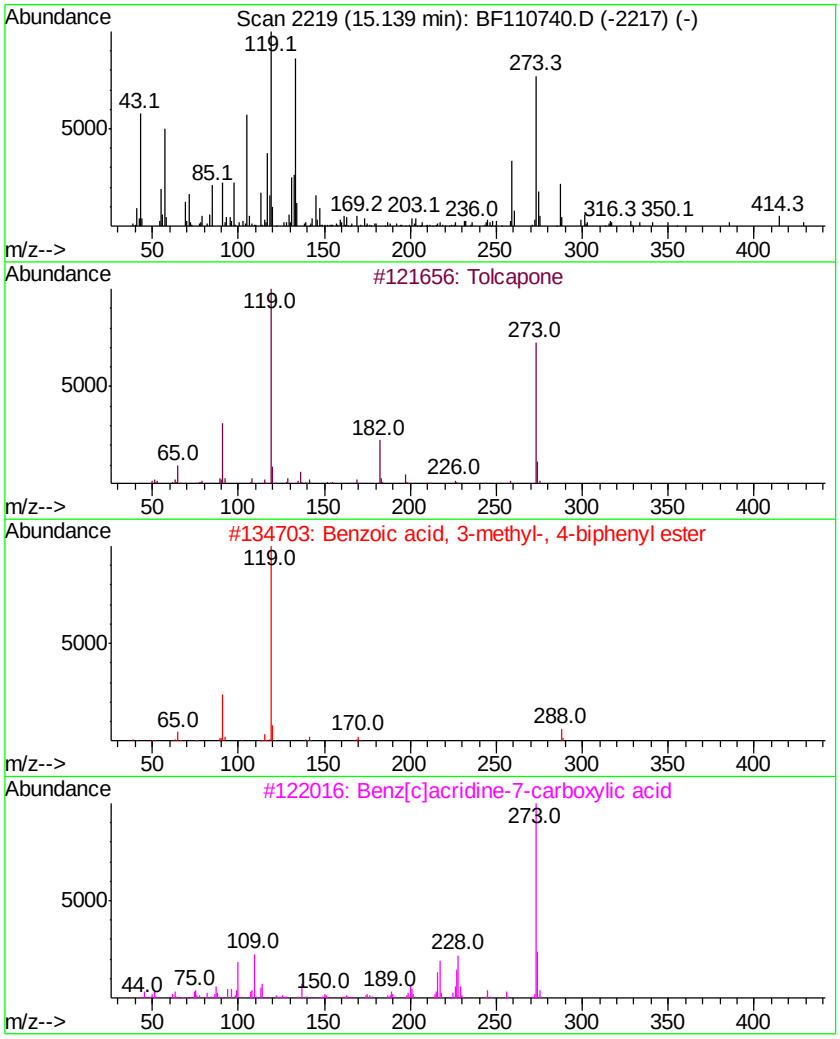
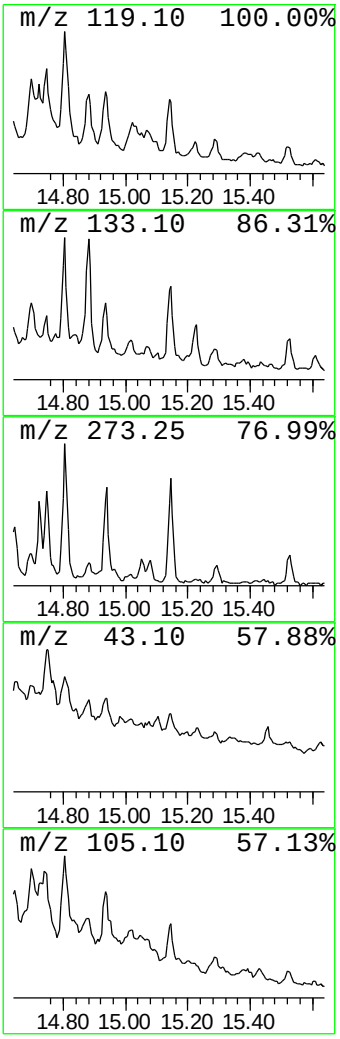
Peak Number 14 unknown15.14 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	45.02 ng	400086	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tolcapone	273	C14H11NO5	134308-13-7	35
2	Benzoic acid, 3-methyl-, 4-biphe...	288	C20H16O2	1000355-71-6	11
3	Benz[c]acridine-7-carboxylic acid	273	C18H11NO2	034623-43-3	11
4	m-Toluic acid, 4-chlorophenyl ester	246	C14H11ClO2	1000307-56-6	11
5	3,3,6,6,9-Pentamethyl-3,4,5,6,7,...	288	C18H24O3	019225-63-9	11





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Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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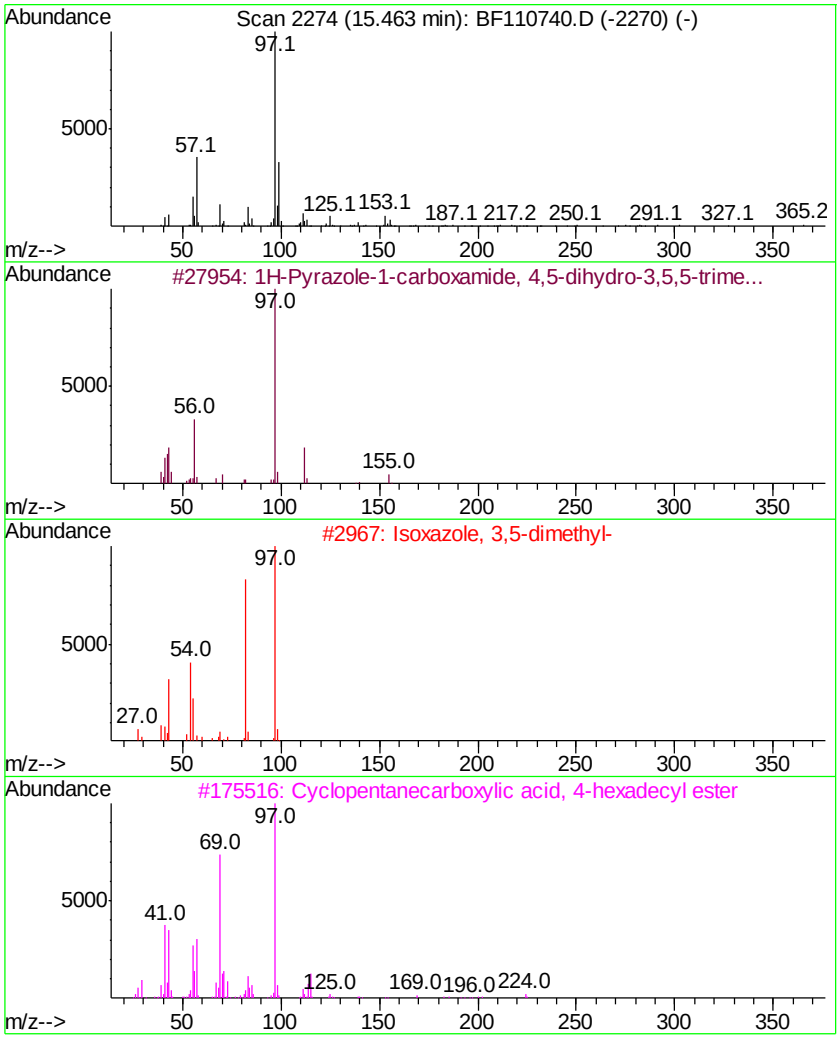
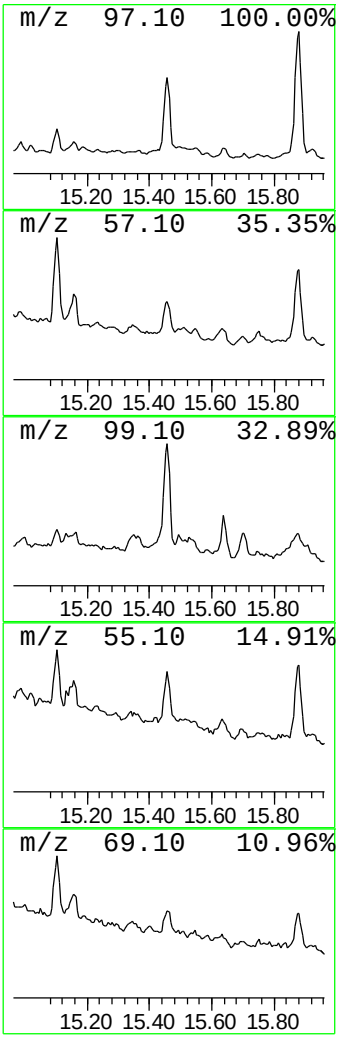
Peak Number 15 1H-Pyrazole-1-carboxamide, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	45.08 ng	400624	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-1-carboxamide, 4,5-d...	155	C7H13N3O	003786-02-5	53
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
3	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	45
4	2-Thiophenylacetic acid, 2-fluor...	236	C12H9FO2S	1000325-71-6	42
5	2-Thiopheneacetic acid, 2-methyl...	198	C10H14O2S	1000278-95-4	42





Library Search Compound Report

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Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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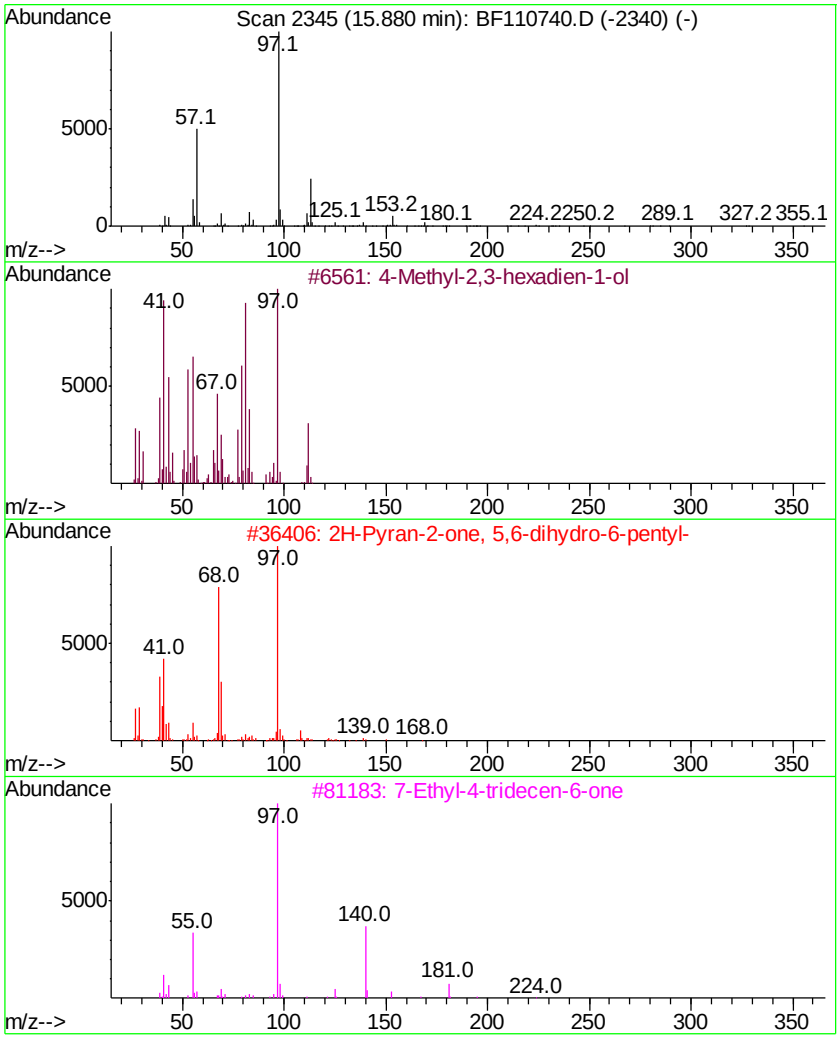
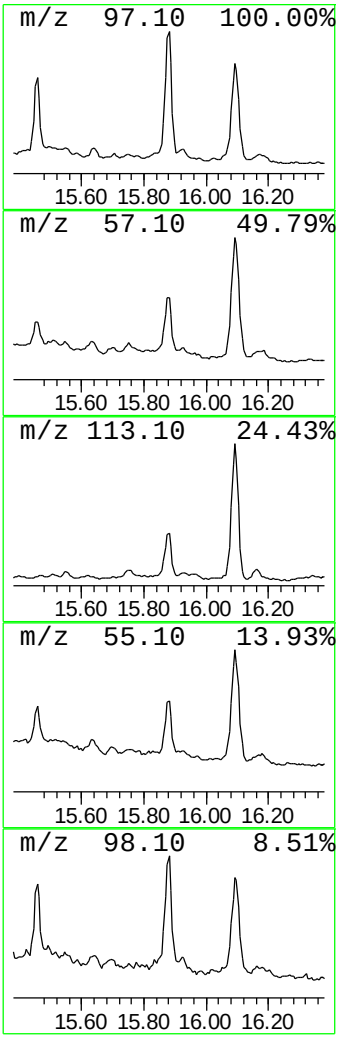
Peak Number 16 unknown15.88 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	78.20 ng	694928	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	49
2	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	47
3	7-Ethyl-4-tridecen-6-one	224	C15H28O	1000374-07-1	45
4	1,2,4-Oxadiazol-5-amine, 3-(4-am...	264	C9H8N6O2S	1000351-26-9	40
5	2-Thiophenemethanethiol	130	C5H6S2	006258-63-5	38





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Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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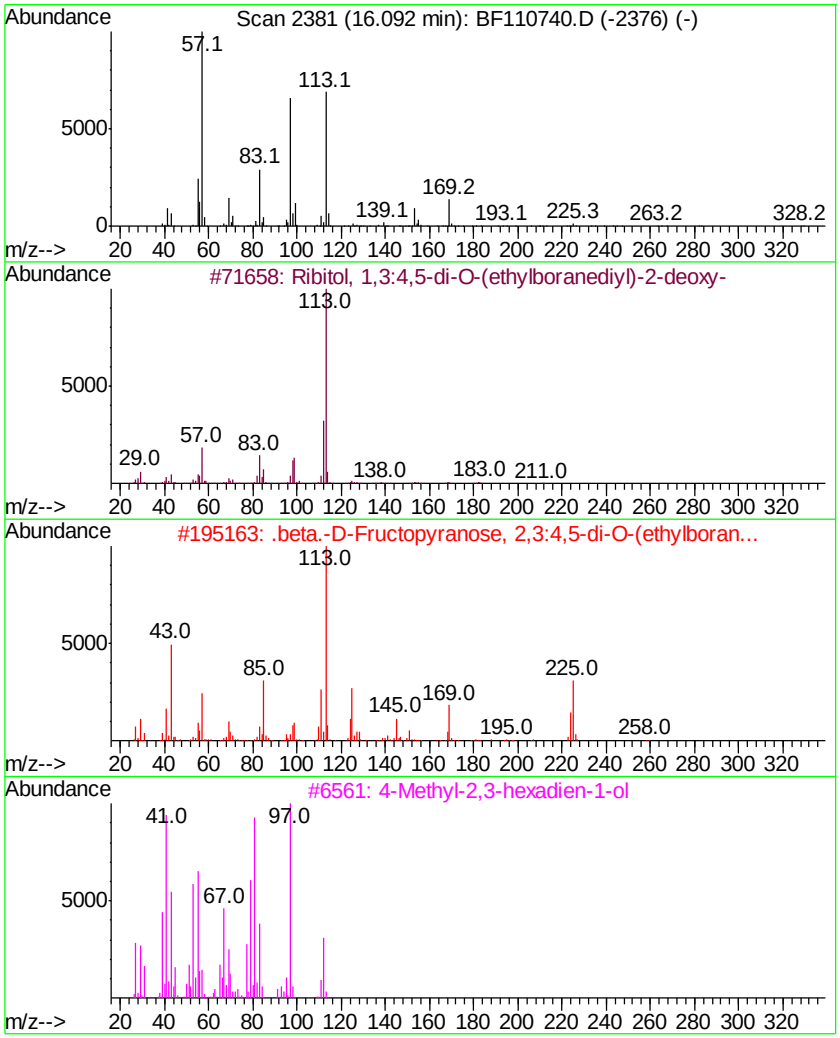
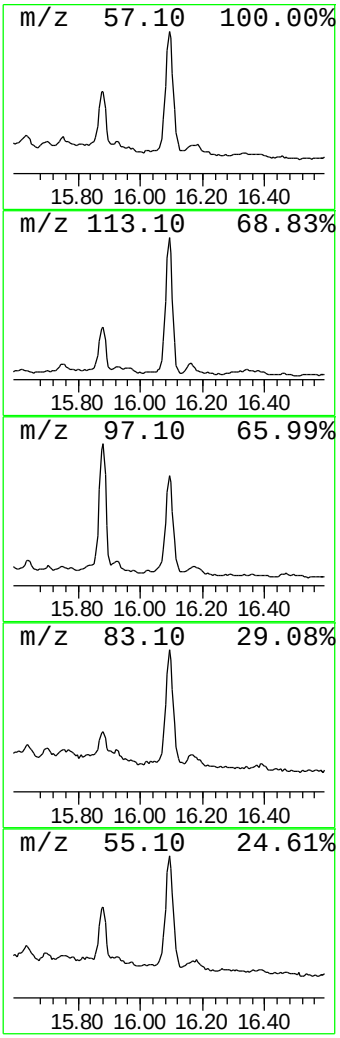
Peak Number 17 unknown16.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	184.44 ng	1639060	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4	1000149-52-8	35
2	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	27
3	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	22
4	Silane, dichlorocyclohexylmethyl-	196	C7H14Cl2Si	005578-42-7	18
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	16





Library Search Compound Report

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Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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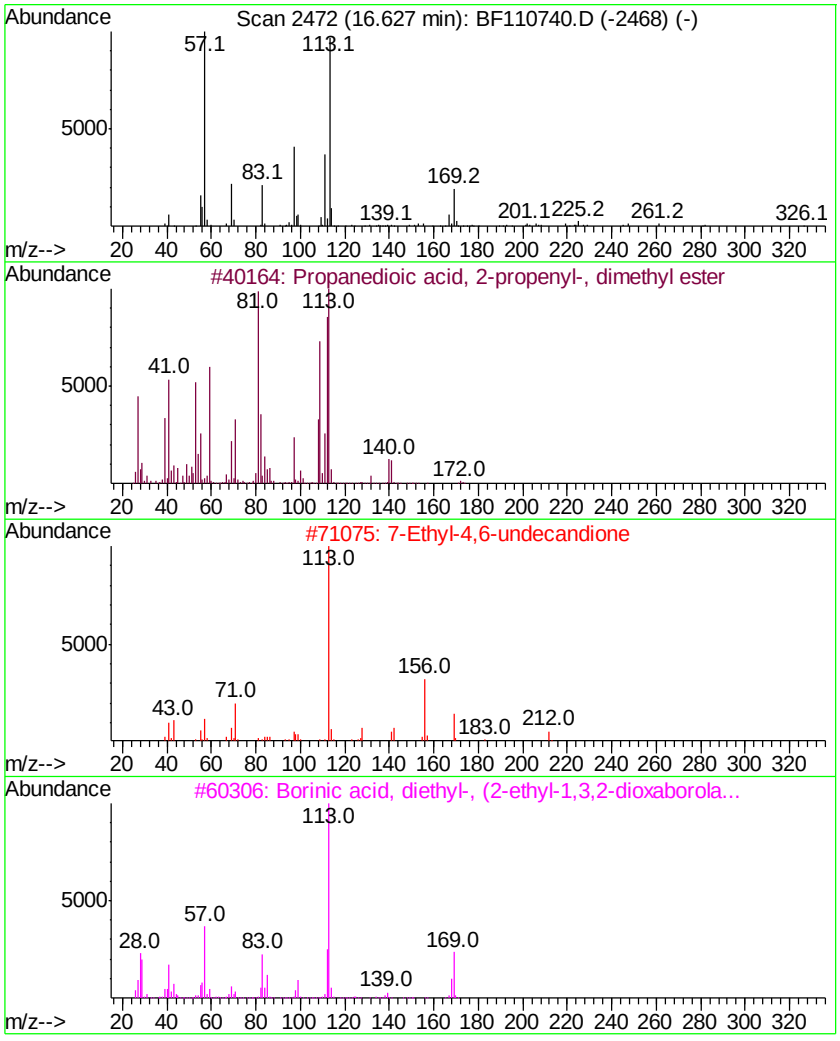
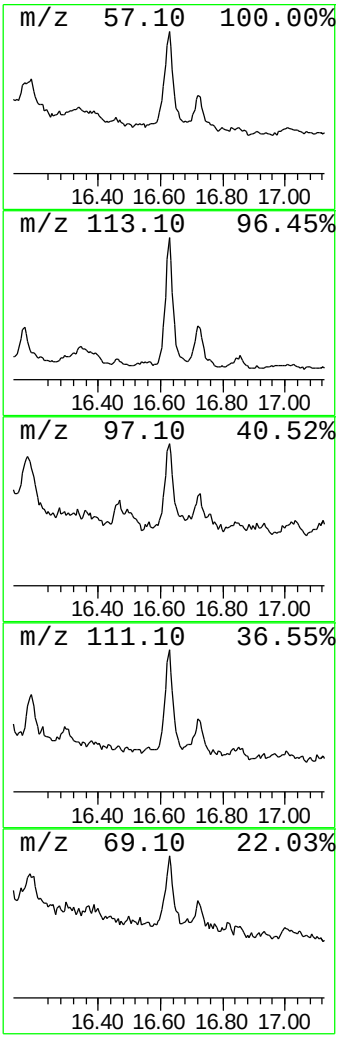
Peak Number 18 unknown16.63 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	39.61 ng	352048	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	38
2	7-Ethyl-4,6-undecandione	212	C13H24O2	1000374-11-8	37
3	Borinic acid, diethyl-, (2-ethyl...	198	C9H20B2O3	058163-56-7	28
4	Acetamide, 2-(4-methyl-1-piperaz...	267	C13H18ClN3O	296245-55-1	27
5	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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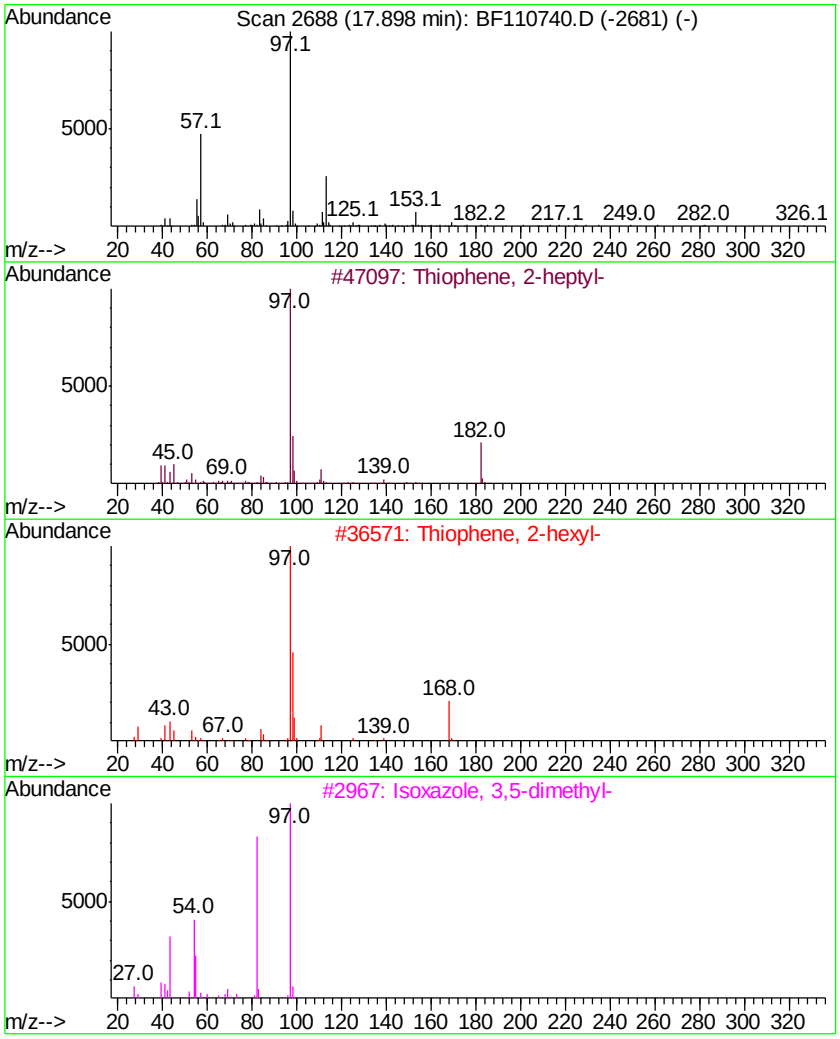
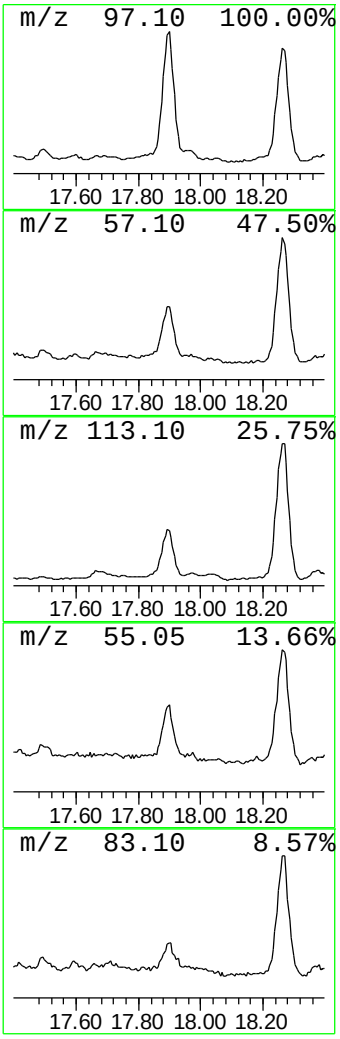
Peak Number 19 Thiophene, 2-heptyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	60.67 ng	539199	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-heptyl-	182	C11H18S	018794-78-0	52
2	Thiophene, 2-hexyl-	168	C10H16S	018794-77-9	50
3	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	50
4	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	47
5	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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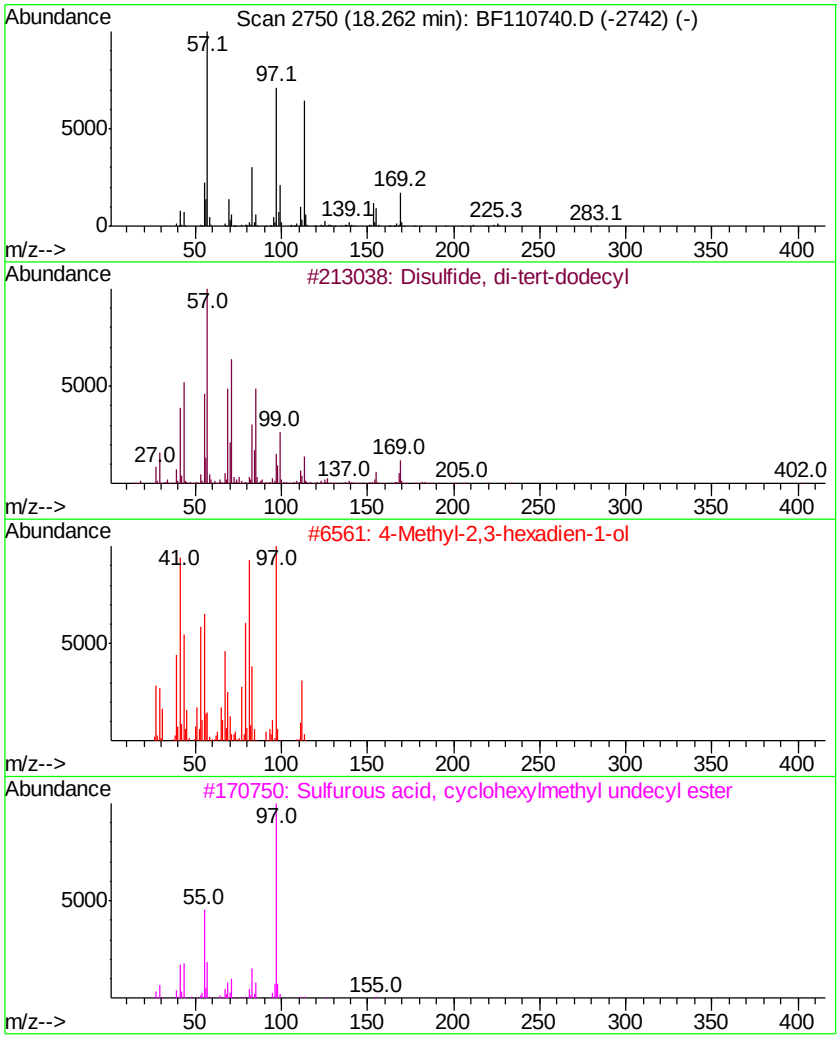
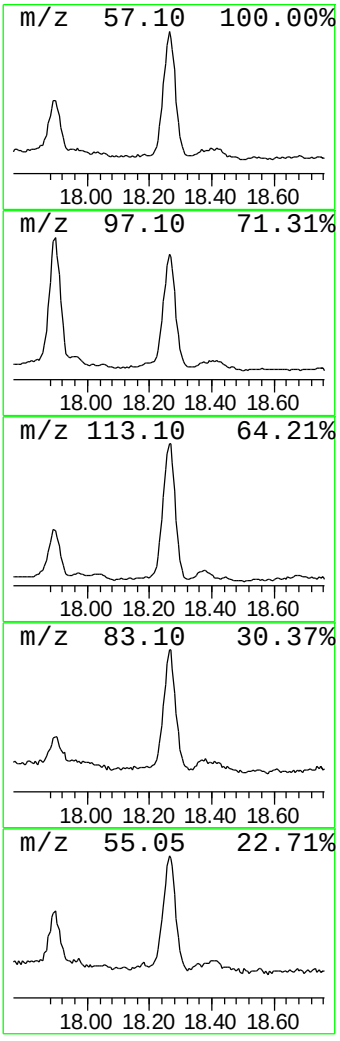
Peak Number 20 unknown18.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	148.57 ng	1320310	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	47
2	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	25
3	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	22
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	22
5	Cyclohexanecarboxylic acid, 2-et...	184	C10H16O3	113122-03-5	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111318\
Data File : BF110740.D
Acq On : 14 Nov 2018 00:56
Operator : JU/SJ
Sample : J5921-02 20X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-TANK1-N29675

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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
Sulfurous acid, c...	10.85	35.5	ng	628694	4	11.48	354036	20.0
Sulfurous acid, c...	10.97	38.2	ng	676088	4	11.48	354036	20.0
unknown11.11	11.11	34.7	ng	614241	4	11.48	354036	20.0
Benzene, (1-methy...	11.85	41.8	ng	740250	4	11.48	354036	20.0
Sulfurous acid, c...	11.92	36.0	ng	637376	4	11.48	354036	20.0
unknown12.27	12.27	75.6	ng	1338090	4	11.48	354036	20.0
unknown12.49	12.49	31.6	ng	558475	4	11.48	354036	20.0
7-Ethyl-4-tridece...	14.61	25.9	ng	1182820	5	14.13	913988	20.0
unknown15.10	15.10	51.7	ng	459287	6	15.67	177736	20.0
unknown15.14	15.14	45.0	ng	400086	6	15.67	177736	20.0
1H-Pyrazole-1-car...	15.46	45.1	ng	400624	6	15.67	177736	20.0
unknown15.88	15.88	78.2	ng	694928	6	15.67	177736	20.0
unknown16.09	16.09	184.4	ng	1639060	6	15.67	177736	20.0
unknown16.63	16.63	39.6	ng	352048	6	15.67	177736	20.0
Thiophene, 2-heptyl-	17.90	60.7	ng	539199	6	15.67	177736	20.0
unknown18.26	18.26	148.6	ng	1320310	6	15.67	177736	20.0