LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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	501	505	511	rBV	65014	69758	3.40%	0.216%
2	5.487	574	578	592	rBV	1725486	1684965	82.18%	5.224%
3	6.498	746	750	765	rBV	1972844	1930006	94.13%	5.984%
4	6.628	769	772	780	rVV	2162401	1923429	93.81%	5.963%
5	6.857	807	811	818	rBV	1582596	1366132	66.63%	4.235%
6	7.010	833	837	841	rBV	1735105	1479294	72.15%	4.586%
7	7.416	902	906	916	rVB	1185398	1098326	53.57%	3.405%
8	7.880	978	985	988	rBV4	28001	28424	1.39%	0.088%
9	8.139	1025	1029	1032	rBV	2074889	1736629	84.70%	5.384%
10	8.851	1147	1150	1153	rBV	79594	73762	3.60%	0.229%
11	8.951	1163	1167	1170	rBV	64404	62753	3.06%	0.195%
12	9.086	1186	1190	1195	rBV4	19889	25647	1.25%	0.080%
13	9.210	1207	1211	1221	rBV	2444424	2050295	100.00%	6.356%
14	9.316	1227	1229	1233	rVB	27774	31077	1.52%	0.096%
15	9.363	1233	1237	1243	rVB7	34529	58614	2.86%	0.182%
16	9.480	1253	1257	1262	rBV3	34698	55769	2.72%	0.173%
17	9.527	1262	1265	1267	rBV2	53895	54724	2.67%	0.170%
18	9.551	1267	1269	1272	rVV	404731	322655	15.74%	1.000%
19	9.604	1275	1278	1282	rVB	286889	266691	13.01%	0.827%
20	9.651	1282	1286	1288	rBV	104467	94074	4.59%	0.292%
21	9.757	1298	1304	1307	rBV5	36868	73291	3.57%	0.227%
22	9.804	1310	1312	1314	rVV2	37010	26416	1.29%	0.082%
23	9.892	1324	1327	1331	rBV	1947775	1883900	91.88%	5.841%
24	9.922	1331	1332	1336	rVB	200494	153951	7.51%	0.477%
25	9.963	1337	1339	1342	rVB3	38657	42938	2.09%	0.133%
26	10.016	1342	1348	1352	rBV4	193788	264473	12.90%	0.820%
27	10.098	1358	1362	1365	rBV	171549	155583	7.59%	0.482%
28	10.186	1374	1377	1379	rVB2	61516	47098	2.30%	0.146%
29	10.304	1393	1397	1398	rBV4	30460	34474	1.68%	0.107%
30	10.322	1398	1400	1402	rVB2	35747	26604	1.30%	0.082%
31	10.439	1417	1420	1425	rBV	234446	210557	10.27%	0.653%
32	10.533	1433	1436	1439	rVB4	88243	85321	4.16%	0.265%
33	10.563	1439	1441	1444	rVB2	109401	92890	4.53%	0.288%
34	10.598	1444	1447	1449	rBV	52940	49473	2.41%	0.153%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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	10.686	1458	1462	1466	rBV	1267251	1150317	56.10%	3.566%
36	10.804	1478	1482	1489	rVB4	101218	134800	6.57%	0.418%
37	10.992	1511	1514	1516	rBV2	28952	24236	1.18%	0.075%
38	11.045	1521	1523	1525	rBV2	26520	24995	1.22%	0.077%
39	11.098	1530	1532	1534	rBV2	33591	24732	1.21%	0.077%
40	11.186	1544	1547	1550	rVB	40785	37064	1.81%	0.115%
41	11.274	1560	1562	1568	rVB	89172	103829	5.06%	0.322%
42	11.380	1577	1580	1582	rBV	1754411	1603354	78.20%	4.971%
43	11.404	1582	1584	1587	rVV	1240128	1095952	53.45%	3.398%
44	11.427	1587	1588	1591	rVV2	144828	125523	6.12%	0.389%
45	11.457	1591	1593	1596	rVV	333194	257292	12.55%	0.798%
46	11.486	1596	1598	1600	rVV2	37965	36648	1.79%	0.114%
47	11.516	1600	1603	1607	rVB	101568	88488	4.32%	0.274%
48	11.592	1613	1616	1618	rBV3	49575	61127	2.98%	0.190%
49	11.610	1618	1619	1626	rVB	73678	85767	4.18%	0.266%
50	11.727	1636	1639	1642	rVB	97381	82450	4.02%	0.256%
51	11.868	1659	1663	1665	rBV	241863	257778	12.57%	0.799%
52	11.910	1667	1670	1676	rVB2	354699	423006	20.63%	1.311%
53	11.998	1682	1685	1687	rBV2	160202	158404	7.73%	0.491%
54	12.074	1696	1698	1704	rVB4	126415	137408	6.70%	0.426%
55	12.180	1713	1716	1718	rVB	64190	64792	3.16%	0.201%
56	12.210	1718	1721	1723	rVB3	53739	48598	2.37%	0.151%
57	12.268	1728	1731	1733	rVB4	59894	52175	2.54%	0.162%
58	12.310	1735	1738	1740	rBV3	49563	73830	3.60%	0.229%
59	12.357	1744	1746	1749	rBV3	50778	52421	2.56%	0.163%
60	12.415	1753	1756	1760	rBV2	283461	334719	16.33%	1.038%
61	12.515	1770	1773	1779	rBV	616074	639802	31.21%	1.984%
62	12.598	1783	1787	1792	rBV	1193970	1101668	53.73%	3.415%
63	12.692	1800	1803	1806	rBV5	62202	63701	3.11%	0.197%
64	12.827	1820	1826	1832	rVB	870660	907736	44.27%	2.814%
65	12.880	1832	1835	1838	rBV2	78905	79202	3.86%	0.246%
66	12.963	1846	1849	1852	rBV	1690851	1320151	64.39%	4.093%
67	13.157	1879	1882	1886	rVB	130235	164949	8.05%	0.511%
68	13.398	1920	1923	1926	rBV3	266759	242755	11.84%	0.753%
69	13.468	1933	1935	1937	rVB	127441	87701	4.28%	0.272%
70	13.857	1998	2001	2008	rVB2	205094	266720	13.01%	0.827%
71	14.027	2026	2030	2033	rBV2	1601675	1711717	83.49%	5.307%

LSC Area Percent Report

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Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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

72	14.862	2170	2172	2179	rVB	339588	357190	17.42%	1.107%
73	15.127	2215	2217	2220	rBV	244196	247783	12.09%	0.768%
74	15.509	2278	2282	2286	rBV	765332	964401	47.04%	2.990%

Sum of corrected areas: 32255174

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112217.D
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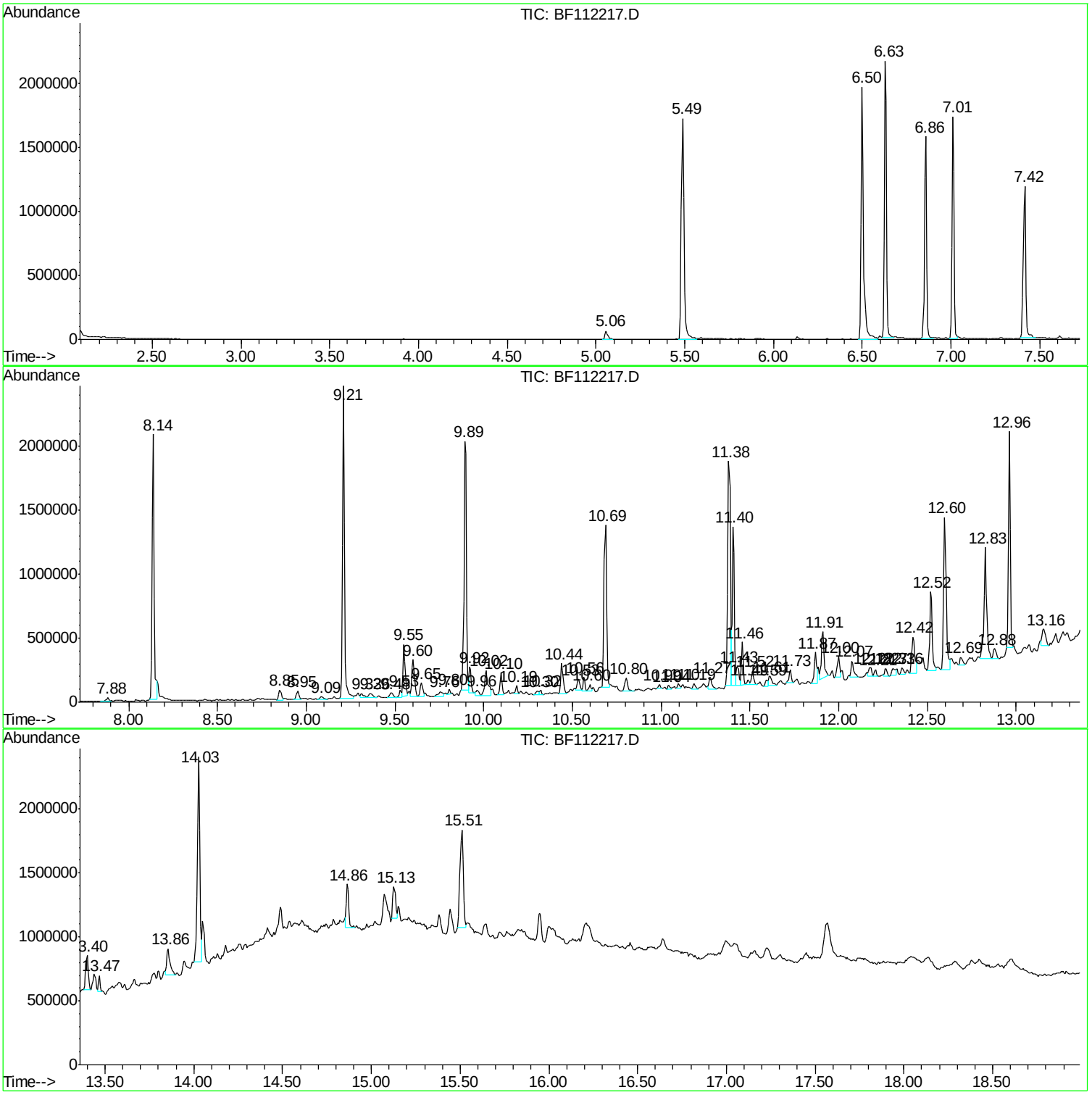
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

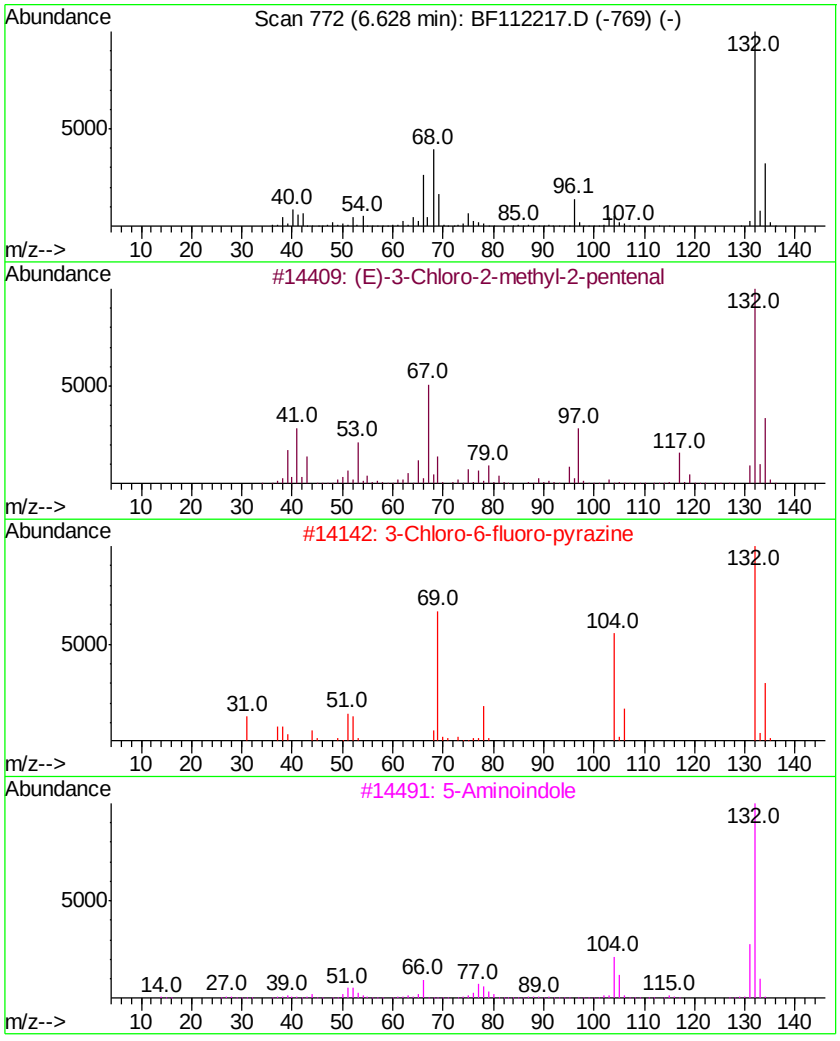
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

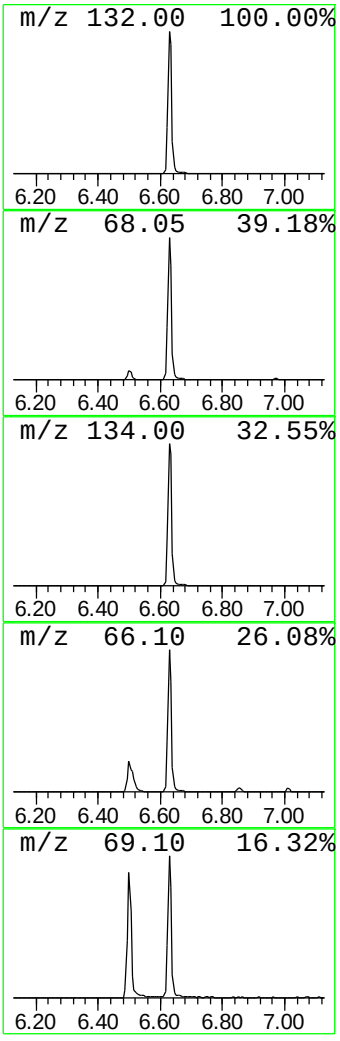
****

Peak Number 1 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	28.16 ng	1923430	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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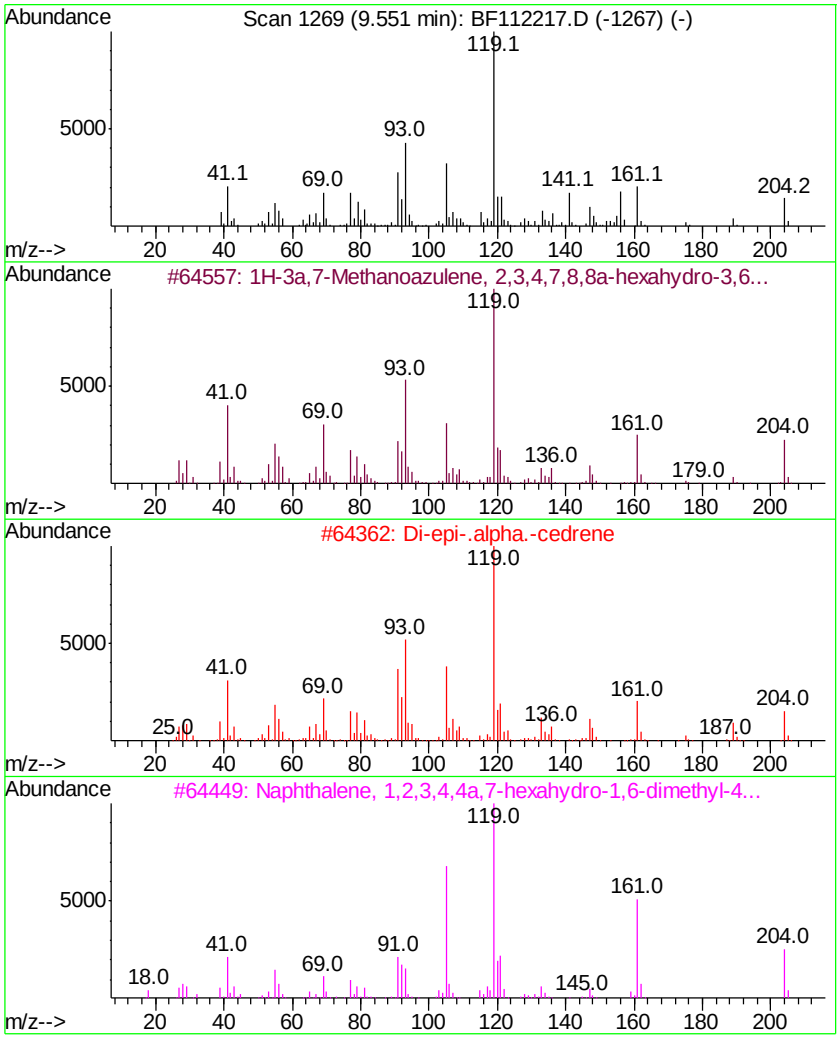
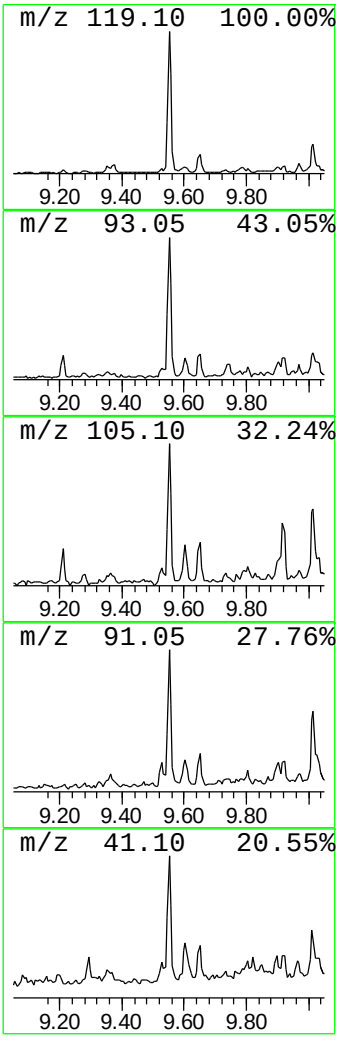
Peak Number 3 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	3.43 ng	322655	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	98
2	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	86
3	Naphthalene, 1,2,3,4,4a,7-hexahy...	204	C15H24	016728-99-7	50
4	Copaene	204	C15H24	003856-25-5	43
5	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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
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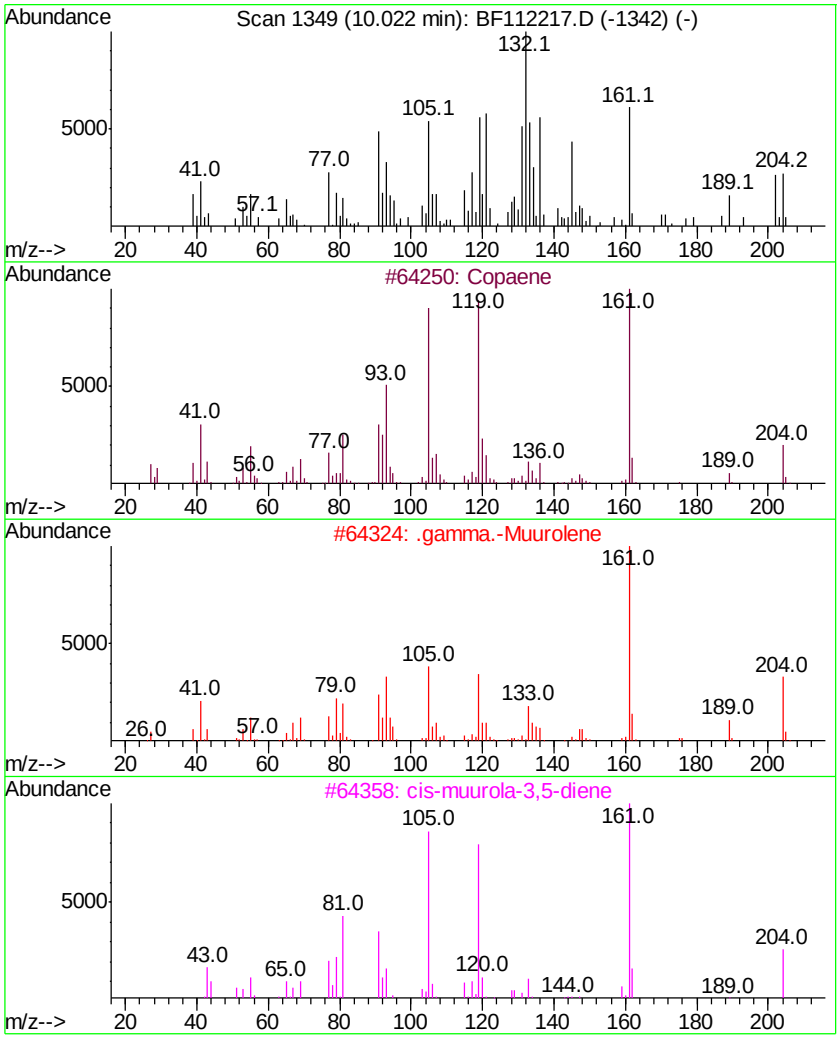
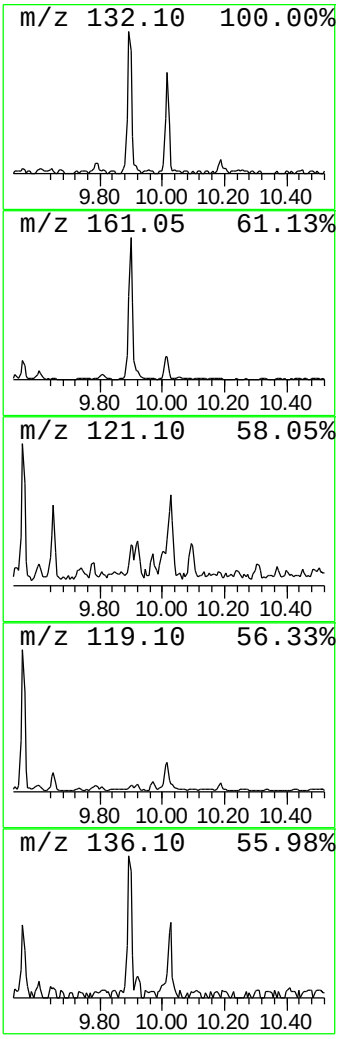
Peak Number 4 Copaene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	2.81 ng	264473	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Copaene	204	C15H24	003856-25-5	84
2	.gamma.-Muurolene	204	C15H24	030021-74-0	68
3	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	60
4	Benzene, 1-(1,5-dimethyl-4-hexen...	202	C15H22	000644-30-4	55
5	Benzene, 1-methyl-4-(1,2,2-trime...	202	C15H22	016982-00-6	55





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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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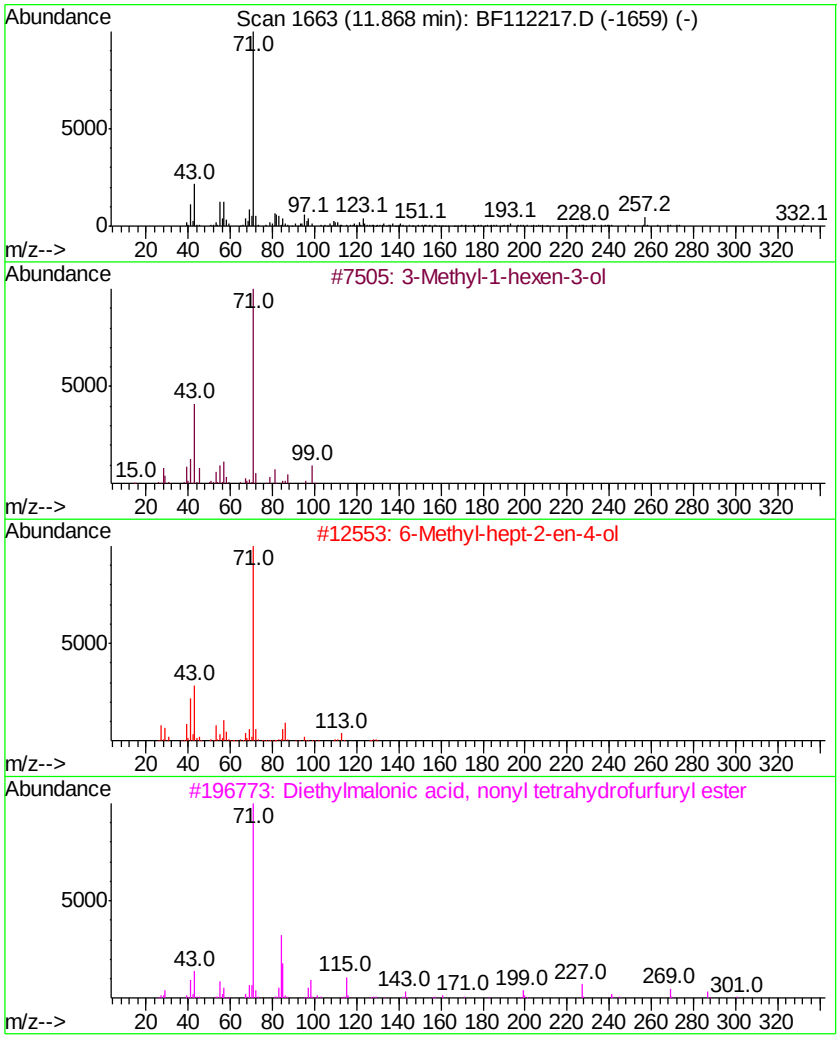
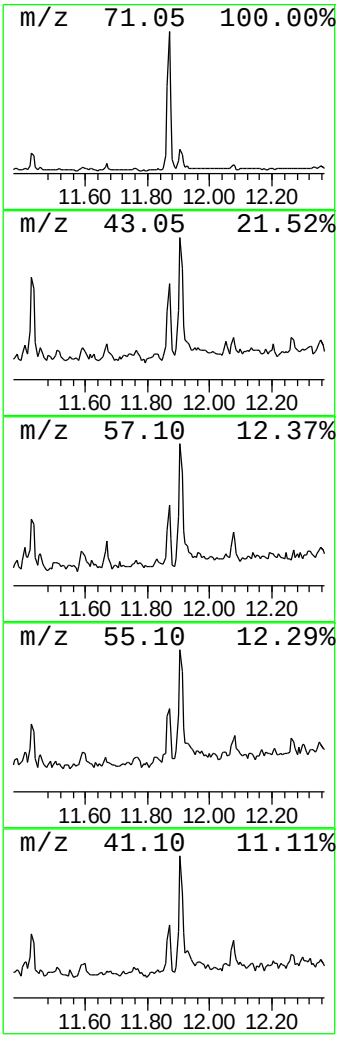
Peak Number 5 3-Methyl-1-hexen-3-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.22 ng	257778	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-1-hexen-3-ol	114	C7H14O	055145-28-3	59
2	6-Methyl-hept-2-en-4-ol	128	C8H16O	083212-30-0	59
3	Diethylmalonic acid, nonyl tetra...	370	C21H38O5	1000370-64-4	53
4	Hexanoic acid, 2-tetrahydrofuryl...	200	C11H20O3	002217-34-7	53
5	Isophytol	296	C20H40O	000505-32-8	53





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Misc :
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Instrument : BNA_F
ClientSampleId : TS-Q

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

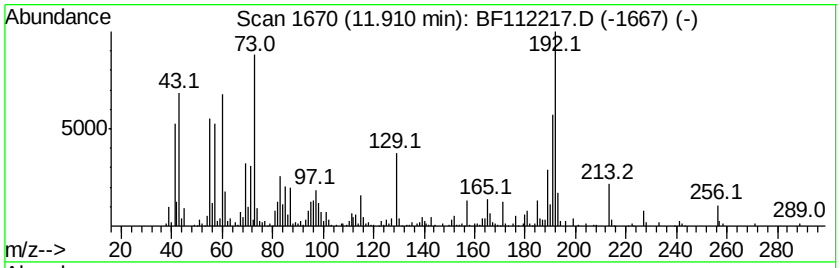
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

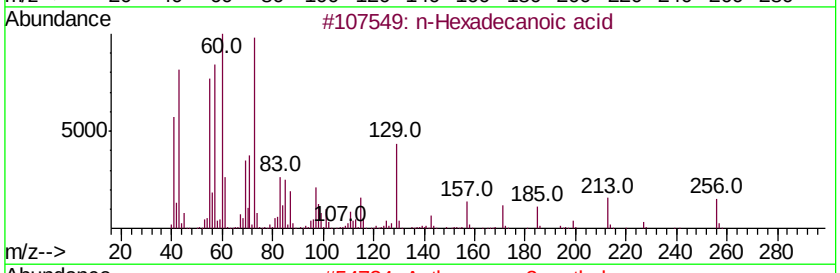
****

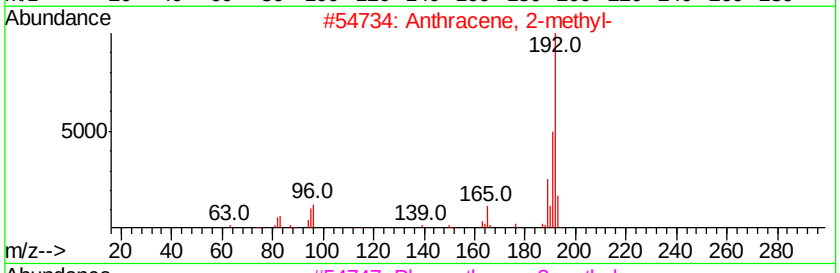
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

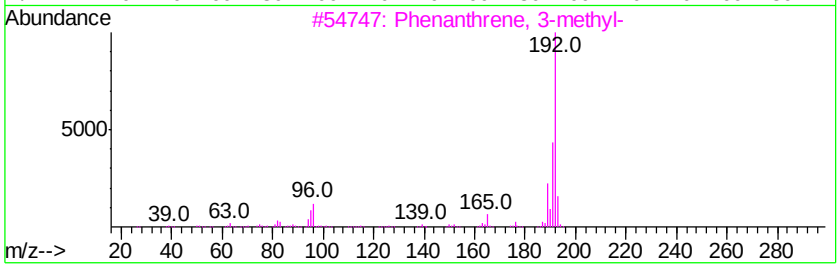
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	5.28 ng	423006	Phenanthrene-d10	11.38

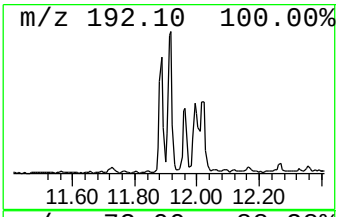
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	86
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	83
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	83

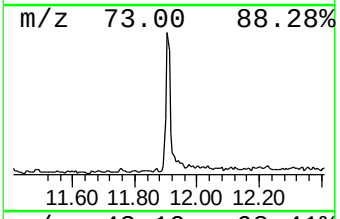


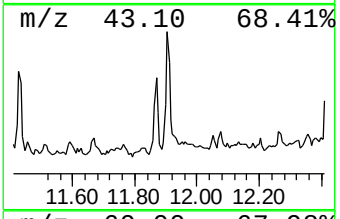


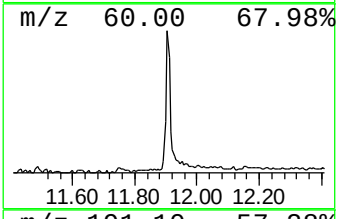


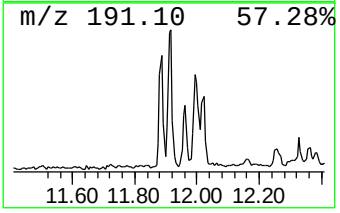












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Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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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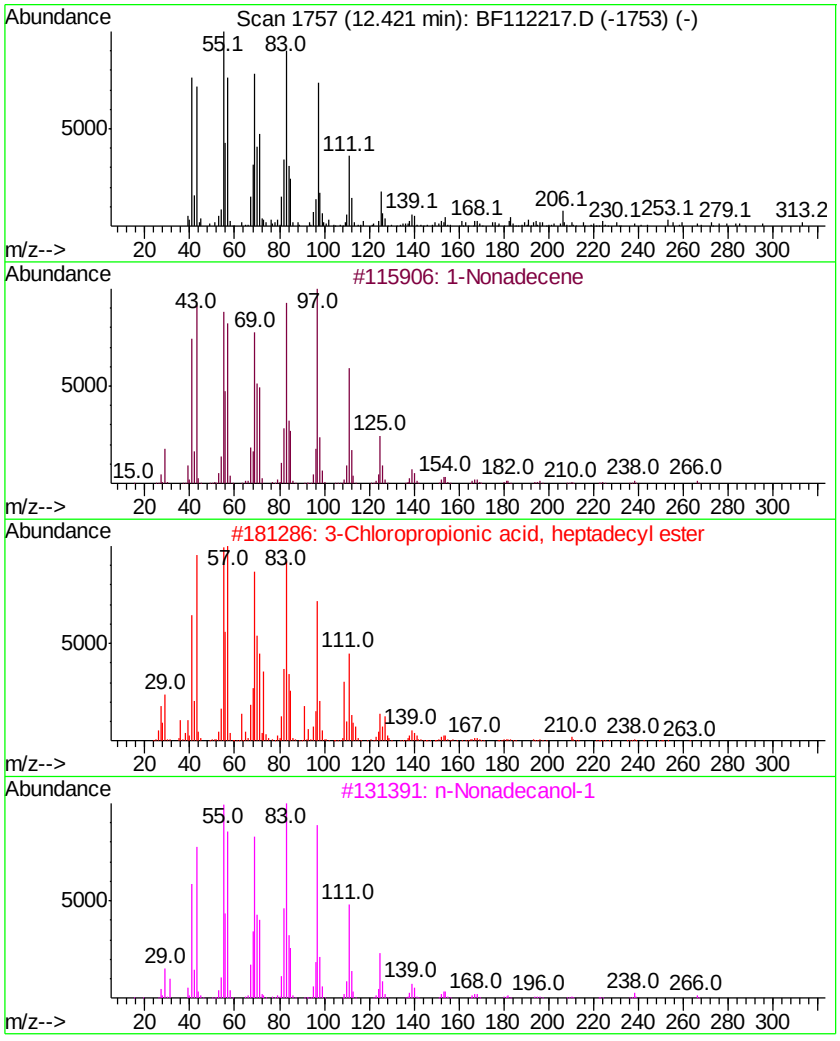
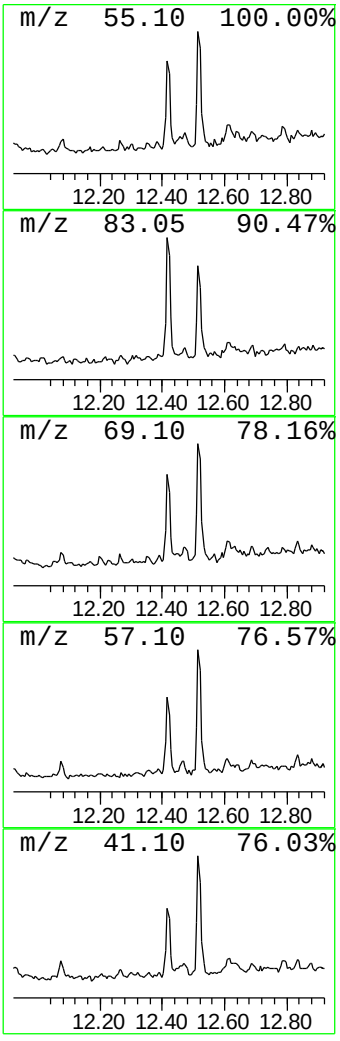
Peak Number 7 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	4.18 ng	334719	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93





Library Search Compound Report

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Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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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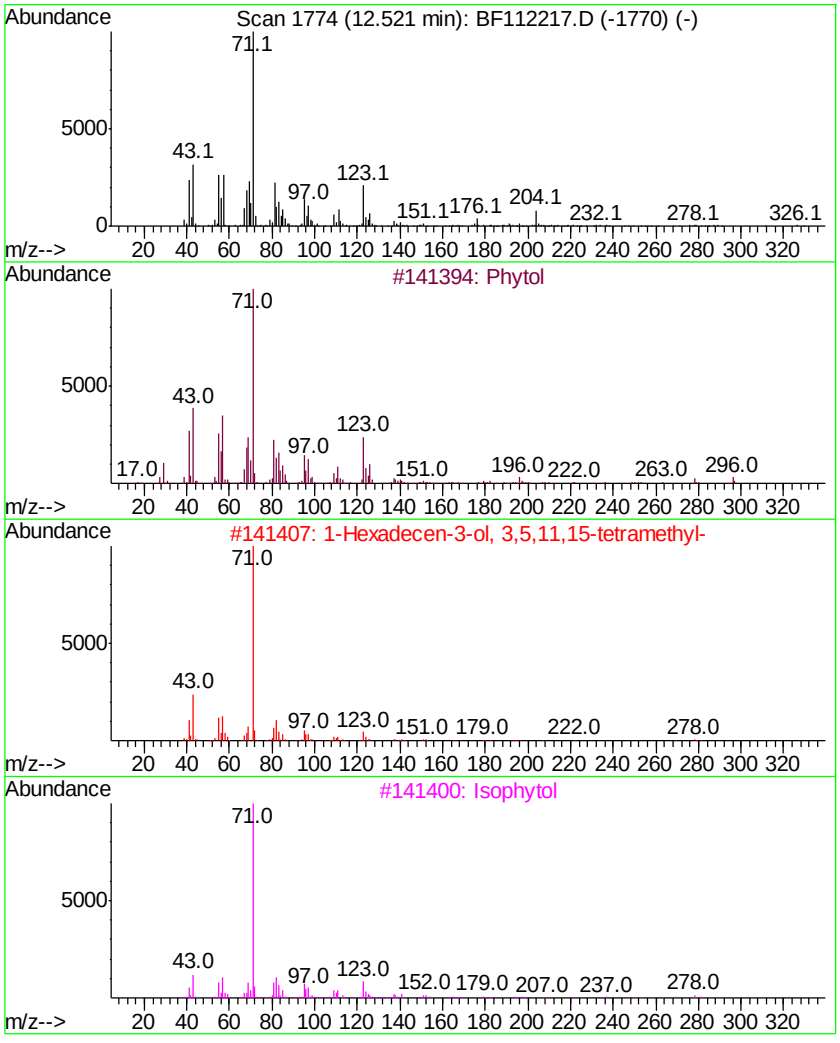
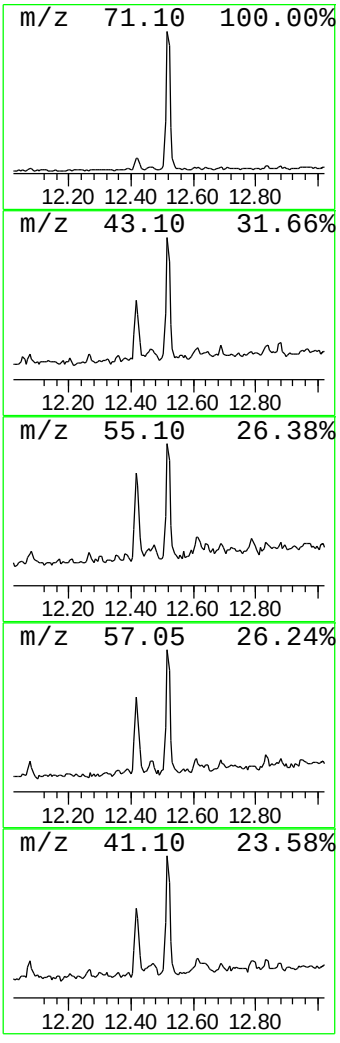
Peak Number 8 Phytol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	7.98 ng	639802	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phytol	296	C20H40O	000150-86-7	93
2	1-Hexadecen-3-ol, 3,5,11,15-tetr...	296	C20H40O	1000262-55-5	64
3	Isophytol	296	C20H40O	000505-32-8	64
4	Butyric acid, 2-pentadecyl ester	298	C19H38O2	107853-73-6	53
5	Butyric acid, 3-pentadecyl ester	298	C19H38O2	1000280-57-3	53





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Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
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TIC Integration Parameters: LSCINT.P

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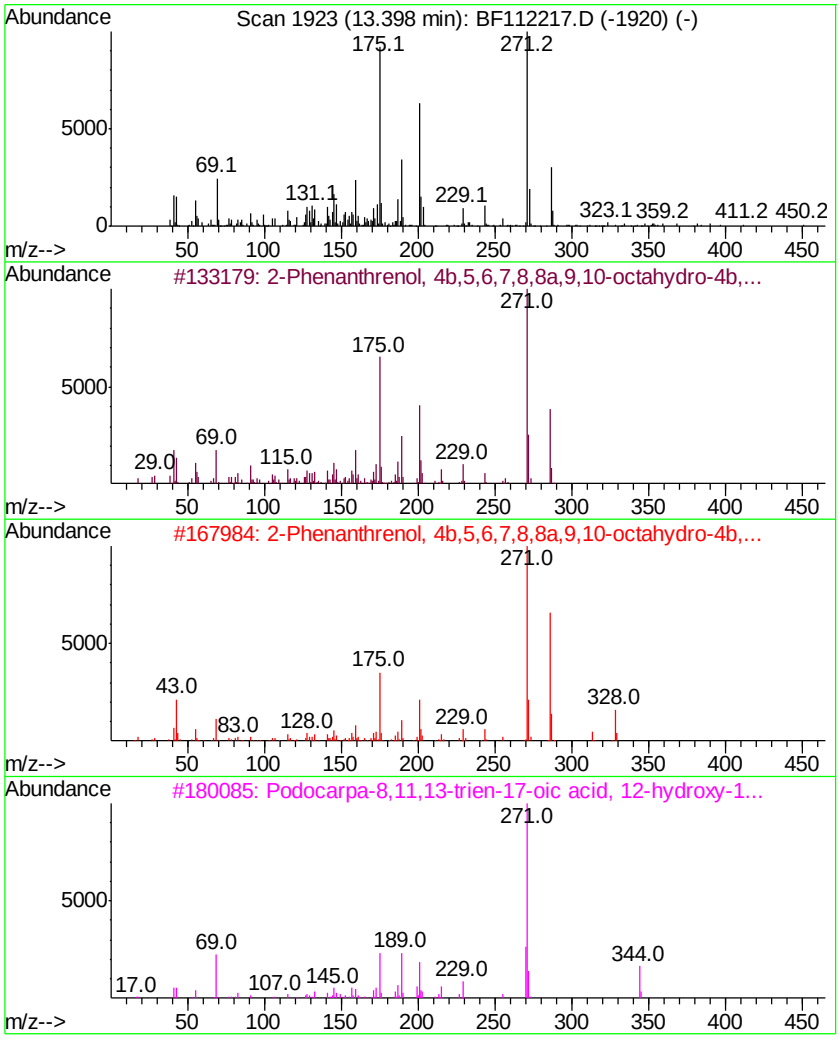
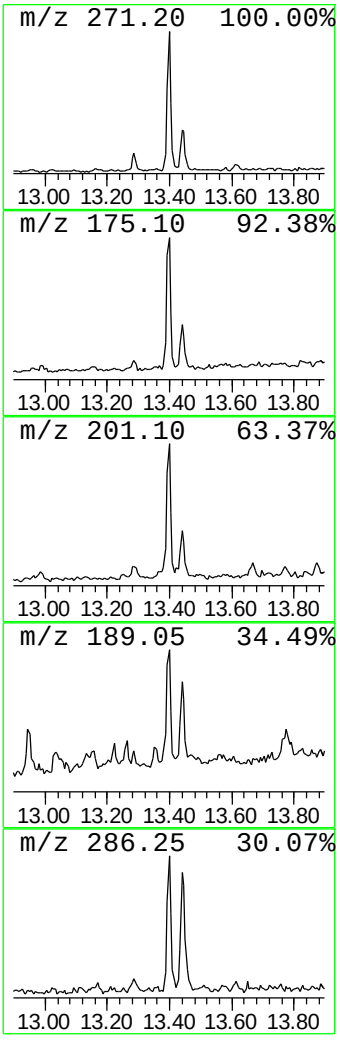
Peak Number 9 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.84 ng	242755	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	60
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	43
3	Podocarpa-8,11,13-trien-17-oic a...	344	C22H32O3	024067-43-4	43
4	Silane, diethylisohexyloxy(trans...	300	C17H36O2Si	1000363-56-5	32
5	Silane, dimethyl(3-methylbut-2-e...	286	C16H34O2Si	1000347-96-9	14





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Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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TIC Library : C:\DATABASE\NIST11.L
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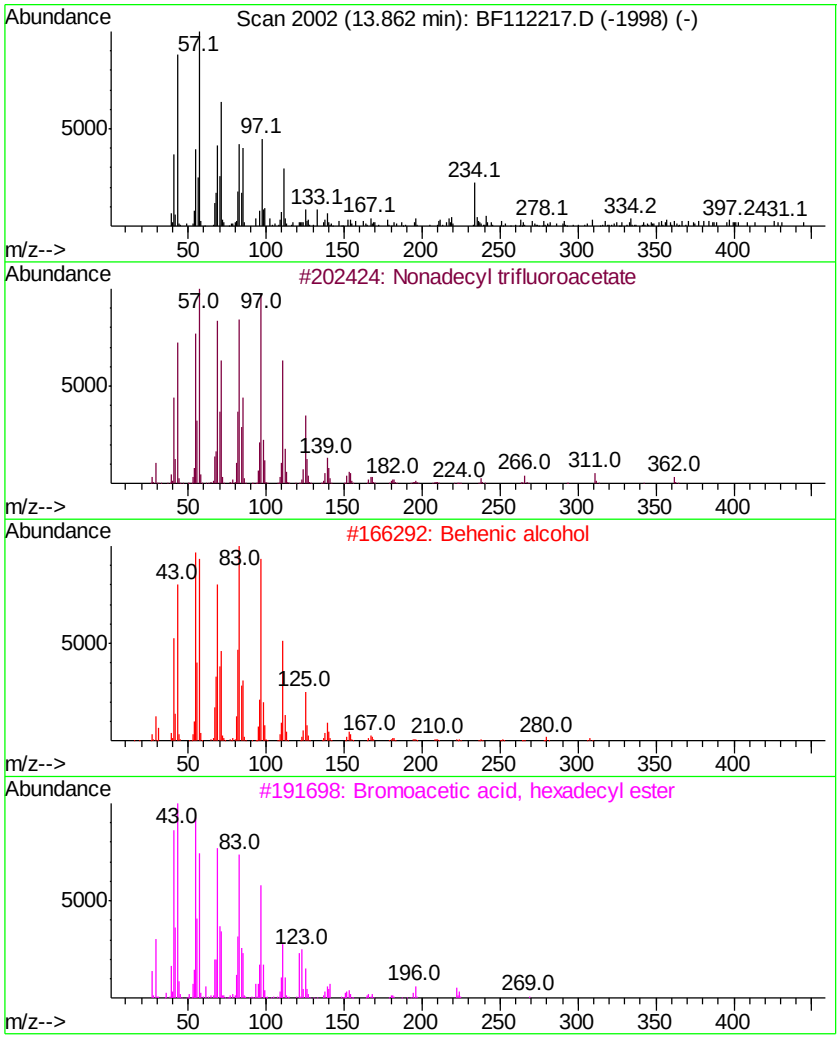
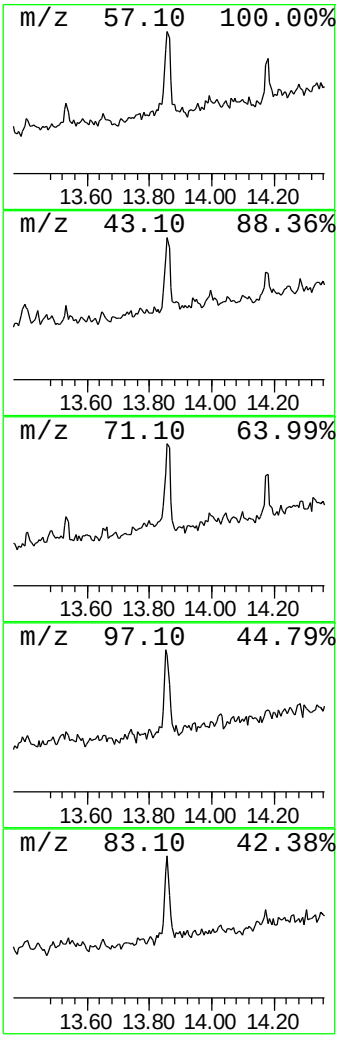
Peak Number 10 Nonadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.12 ng	266720	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
2	Behenic alcohol	326	C22H46O	000661-19-8	81
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	76
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74
5	1-Heptacosanol	396	C27H56O	002004-39-9	74





Library Search Compound Report

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Operator : JU/SJ
Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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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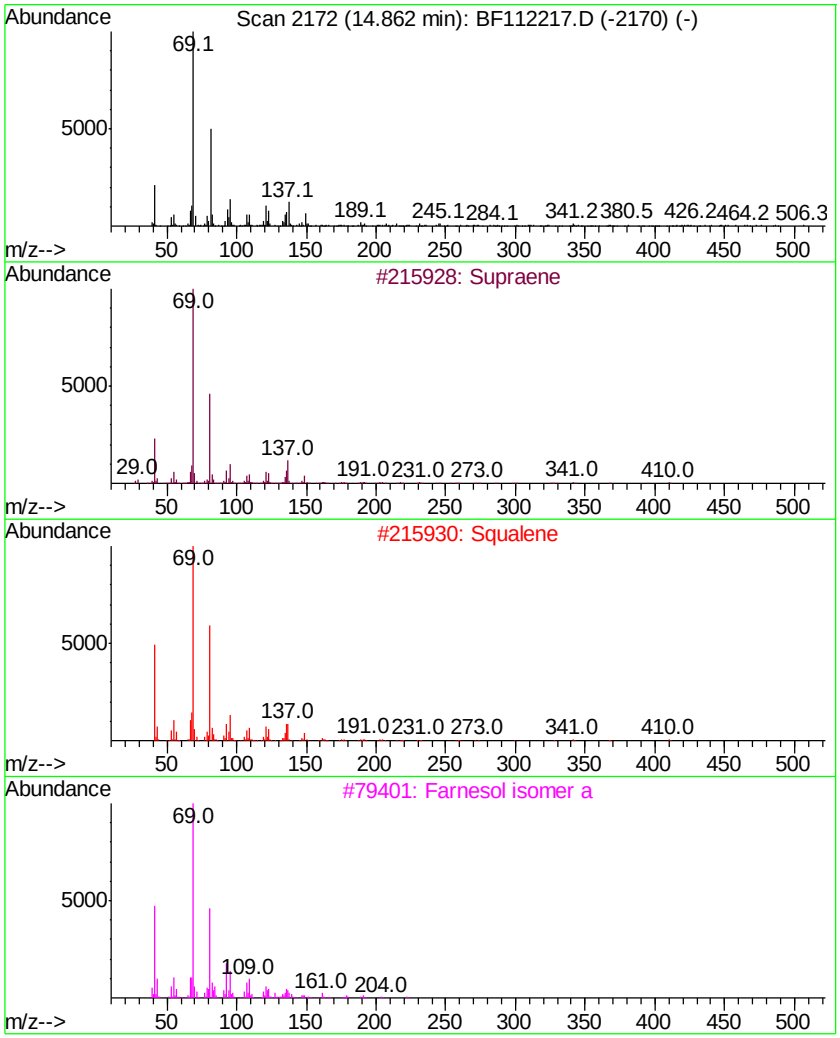
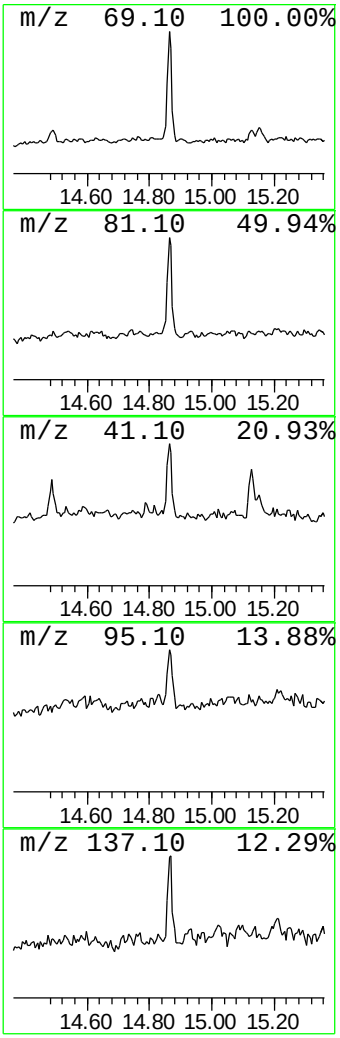
Peak Number 11 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	7.41 ng	357190	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	83
3	Farnesol isomer a	222	C15H26O	1000108-92-4	74
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012419\
Data File : BF112217.D
Acq On : 24 Jan 2019 19:05
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Sample : K1223-05 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-Q

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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	28.2	ng	1923430	1	6.86	1366130	20.0
1H-3a,7-Methanoaz...	9.55	3.4	ng	322655	3	9.89	1883900	20.0
Copaene	10.02	2.8	ng	264473	3	9.89	1883900	20.0
3-Methyl-1-hexen-...	11.87	3.2	ng	257778	4	11.38	1603350	20.0
n-Hexadecanoic acid	11.91	5.3	ng	423006	4	11.38	1603350	20.0
1-Nonadecene	12.42	4.2	ng	334719	4	11.38	1603350	20.0
Phytol	12.52	8.0	ng	639802	4	11.38	1603350	20.0
2-Phenanthrenol, ...	13.40	2.8	ng	242755	5	14.03	1711720	20.0
Nonadecyl trifluo...	13.86	3.1	ng	266720	5	14.03	1711720	20.0
Supraene	14.86	7.4	ng	357190	6	15.51	964401	20.0