LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137343.D
Acq On : 08 Feb 2024 17:50
Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.281	538	543	547	rBV	4048887	4231628	45.34%	8.521%
2	5.416	557	566	573	rBV2	1436363	1992146	21.34%	4.011%
3	5.640	600	604	608	rBV	701562	648489	6.95%	1.306%
4	5.957	649	658	669	rBV2	278477	394600	4.23%	0.795%
5	6.345	721	724	728	rVB	187935	168721	1.81%	0.340%
6	6.416	733	736	742	rBV2	797195	922195	9.88%	1.857%
7	6.469	742	745	748	rVB	377189	325542	3.49%	0.656%
8	6.610	766	769	775	rVB	574601	559128	5.99%	1.126%
9	6.781	795	798	805	rBV	626037	605604	6.49%	1.219%
10	6.839	805	808	814	rVB	368449	315208	3.38%	0.635%
11	6.963	825	829	832	rBV	2539267	2119443	22.71%	4.268%
12	7.039	838	842	848	rBV	486023	428209	4.59%	0.862%
13	7.198	863	869	872	rBV	3621069	4259802	45.64%	8.577%
14	7.351	890	895	901	rVB	2039318	2085065	22.34%	4.198%
15	7.522	920	924	926	rVB2	74792	102891	1.10%	0.207%
16	7.734	956	960	965	rBV	172236	156243	1.67%	0.315%
17	7.816	965	974	975	rBV4	487028	759055	8.13%	1.528%
18	7.834	975	977	985	rVB2	1848845	2071396	22.19%	4.171%
19	8.098	1012	1022	1025	rBV	6781504	9333955	100.00%	18.795%
20	8.139	1025	1029	1035	rVB	1003466	876001	9.39%	1.764%
21	8.875	1143	1154	1156	rBV	1510553	2040974	21.87%	4.110%
22	8.898	1156	1158	1167	rVB	892811	952808	10.21%	1.919%
23	9.145	1194	1200	1203	rBV	3776111	3515787	37.67%	7.079%
24	9.251	1214	1218	1224	rVB2	85194	127262	1.36%	0.256%
25	9.645	1280	1285	1288	rBV2	88043	102667	1.10%	0.207%
26	9.733	1295	1300	1307	rBV3	124299	206580	2.21%	0.416%
27	9.816	1311	1314	1318	rVV2	1092728	1134509	12.15%	2.284%
28	9.851	1318	1320	1324	rVB	222468	172947	1.85%	0.348%
29	10.551	1436	1439	1442	rBV	121763	98107	1.05%	0.198%
30	10.610	1442	1449	1454	rVV	2713112	2979896	31.93%	6.000%
31	10.680	1458	1461	1467	rVB2	101892	151569	1.62%	0.305%
32	11.310	1564	1568	1576	rBV	1020740	861878	9.23%	1.735%
33	11.851	1656	1660	1672	rBV	282275	296943	3.18%	0.598%
34	11.969	1677	1680	1694	rVV	167539	179133	1.92%	0.361%
35	12.910	1836	1840	1844	rBV	3247729	3068262	32.87%	6.178%
36	13.821	1992	1995	2003	rBV	183290	215961	2.31%	0.435%

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Misc :
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Instrument :
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CG-MW-17-ch6

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.963	2015	2019	2025	rBV	645718	589841	6.32%	1.188%
38	15.445	2266	2271	2279	rBV	489263	612136	6.56%	1.233%

Sum of corrected areas: 49662581

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Instrument :
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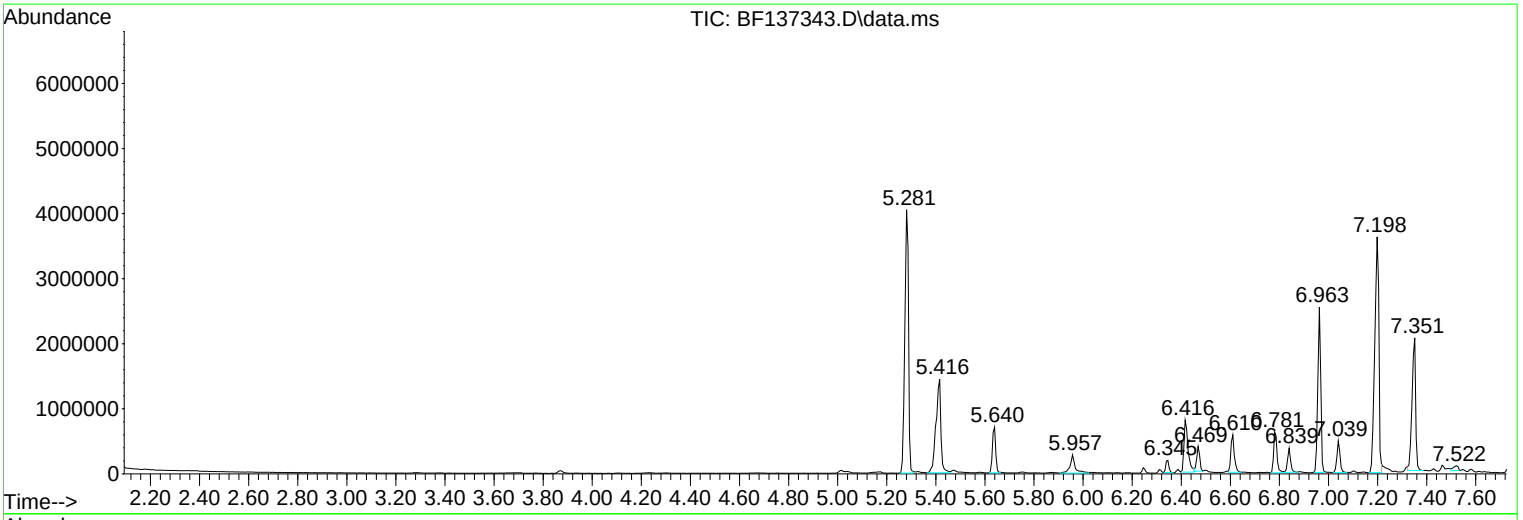
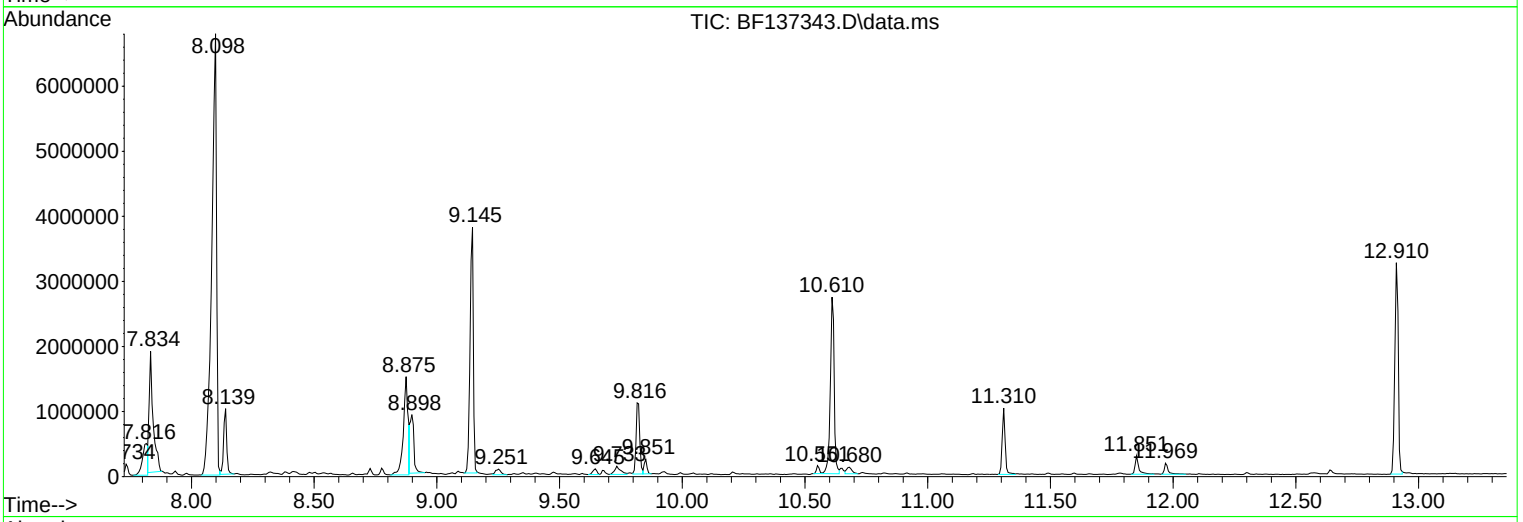
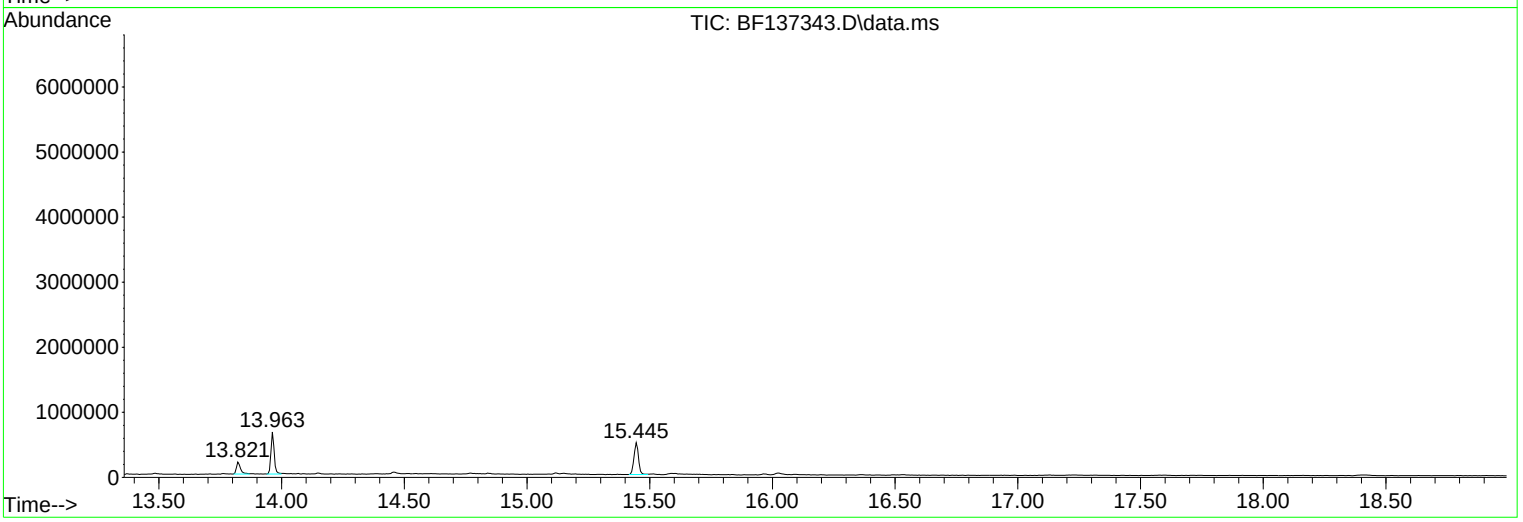
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137343.D
Acq On : 08 Feb 2024 17:50
Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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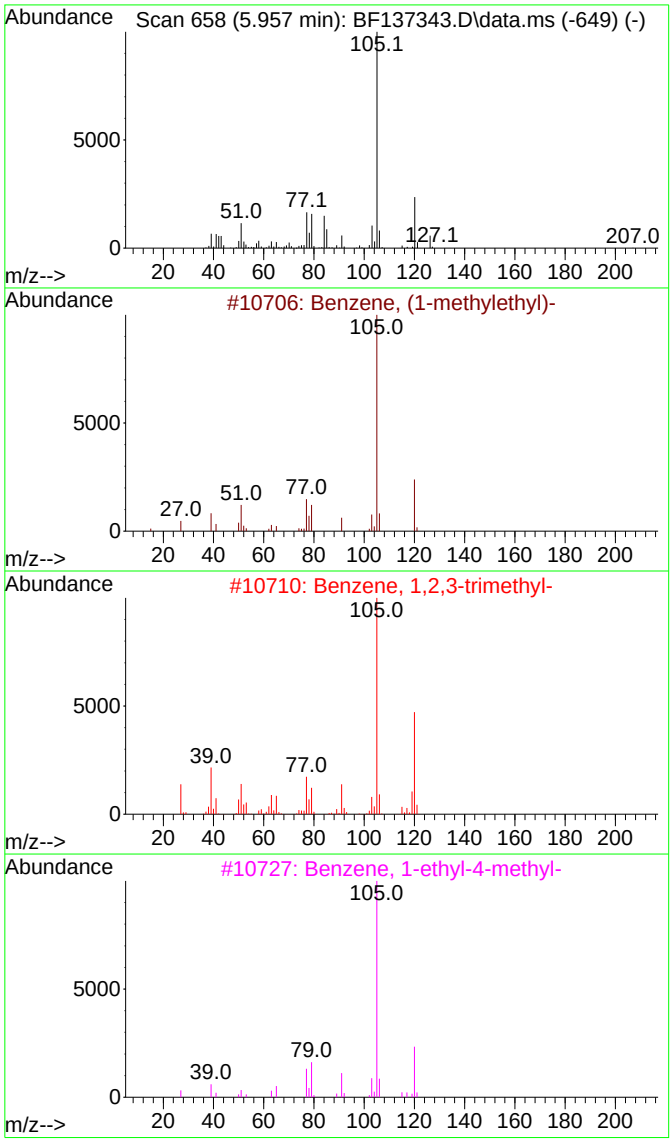
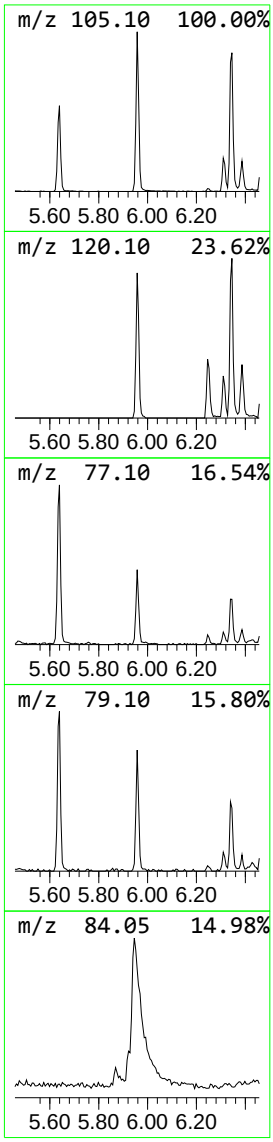
Peak Number 3 Benzene, (1-methylethyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.957	13.03 ng	394600	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	93
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	74
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	58
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	58
5	2,3-Heptadien-5-yne, 2,4-dimethyl-	120	C9H12	041898-89-9	58





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Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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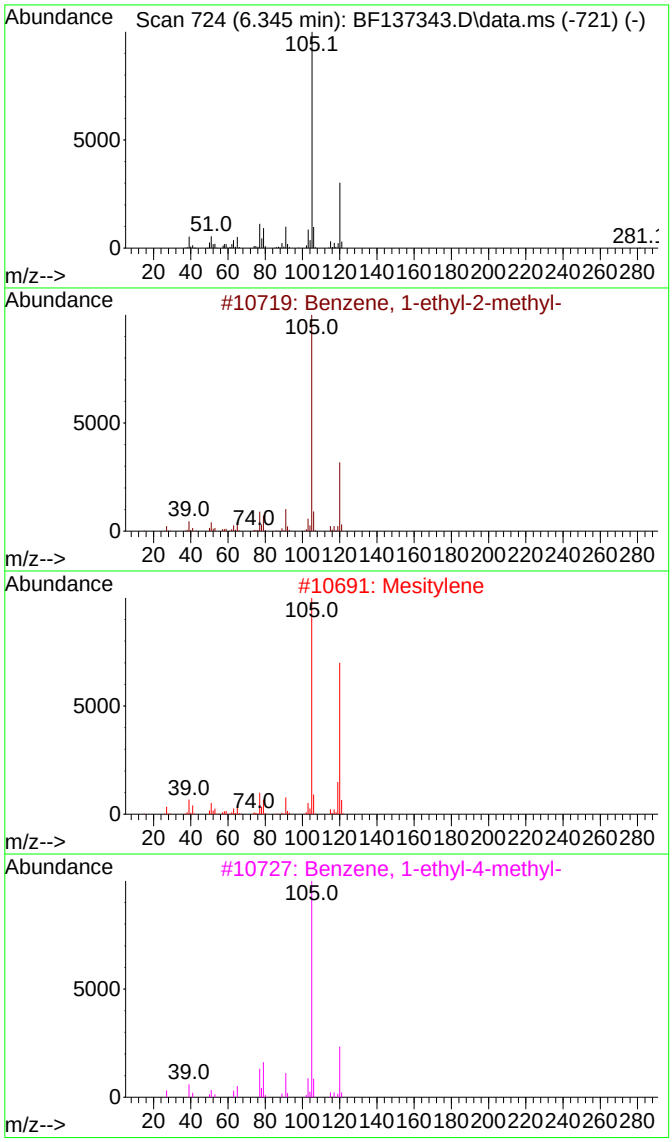
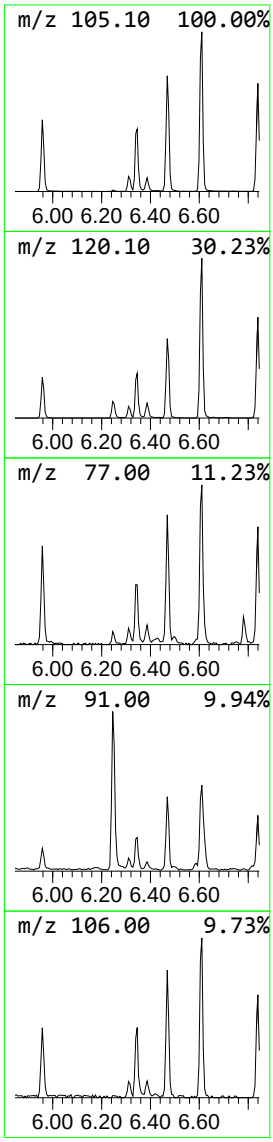
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.345	5.57 ng	168721	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137343.D
Acq On : 08 Feb 2024 17:50
Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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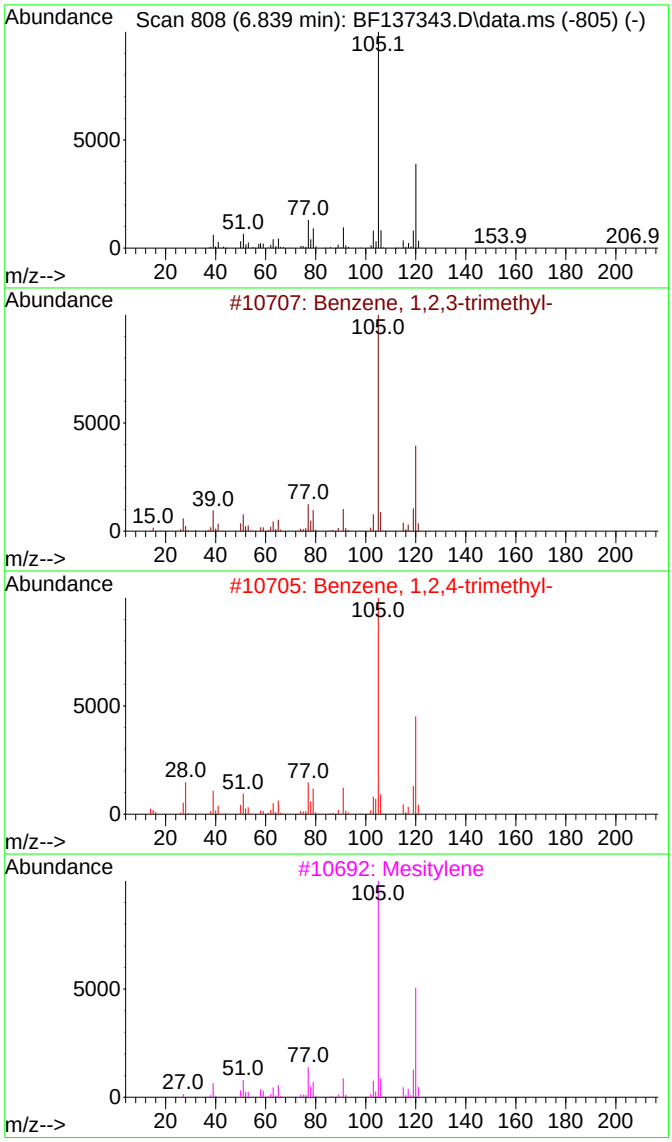
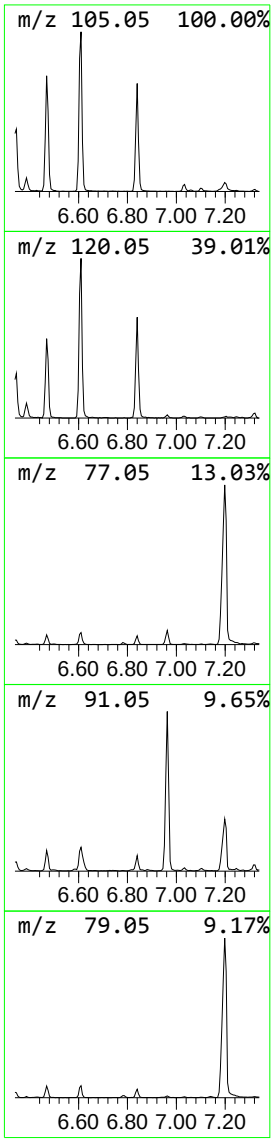
Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.839	10.41 ng	315208	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
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Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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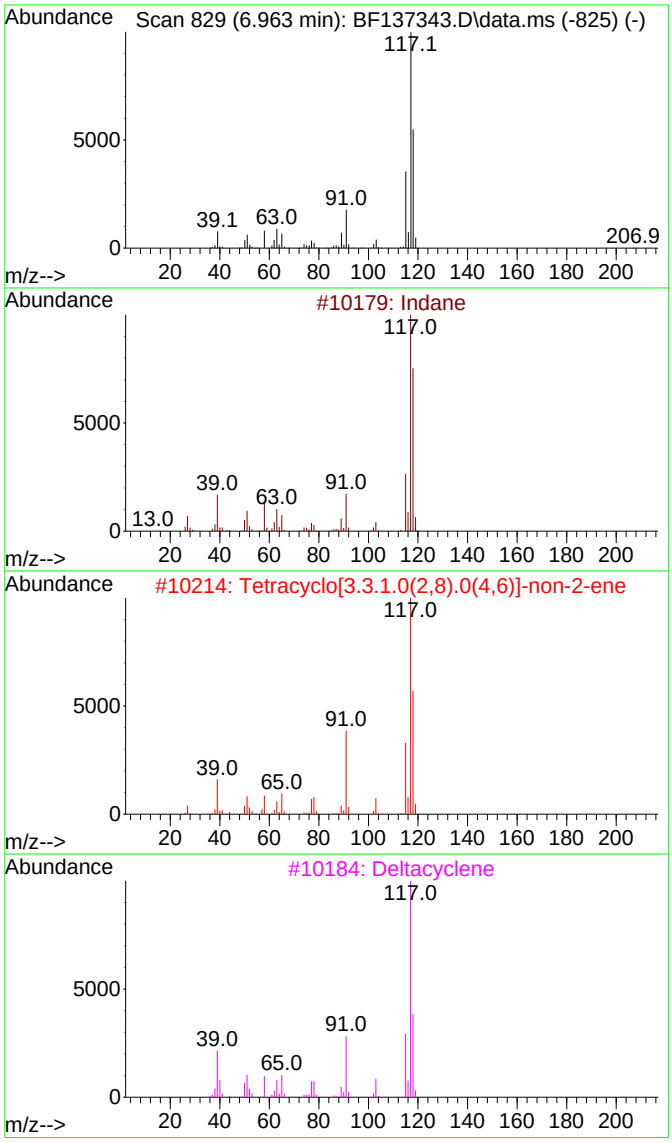
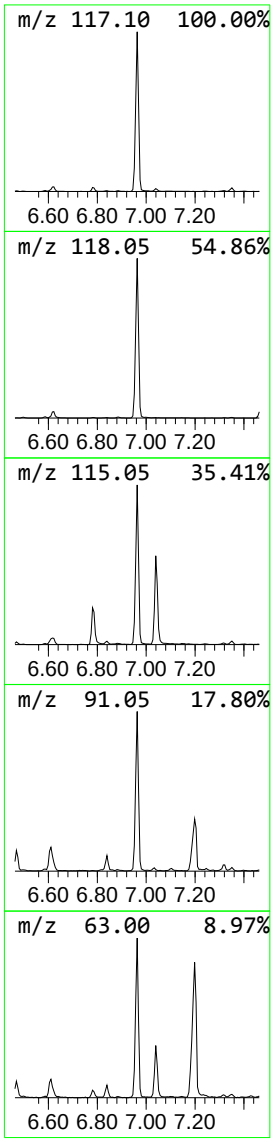
Peak Number 7 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	69.99 ng	2119440	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
3	Deltacyclene	118	C9H10	007785-10-6	64
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137343.D
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Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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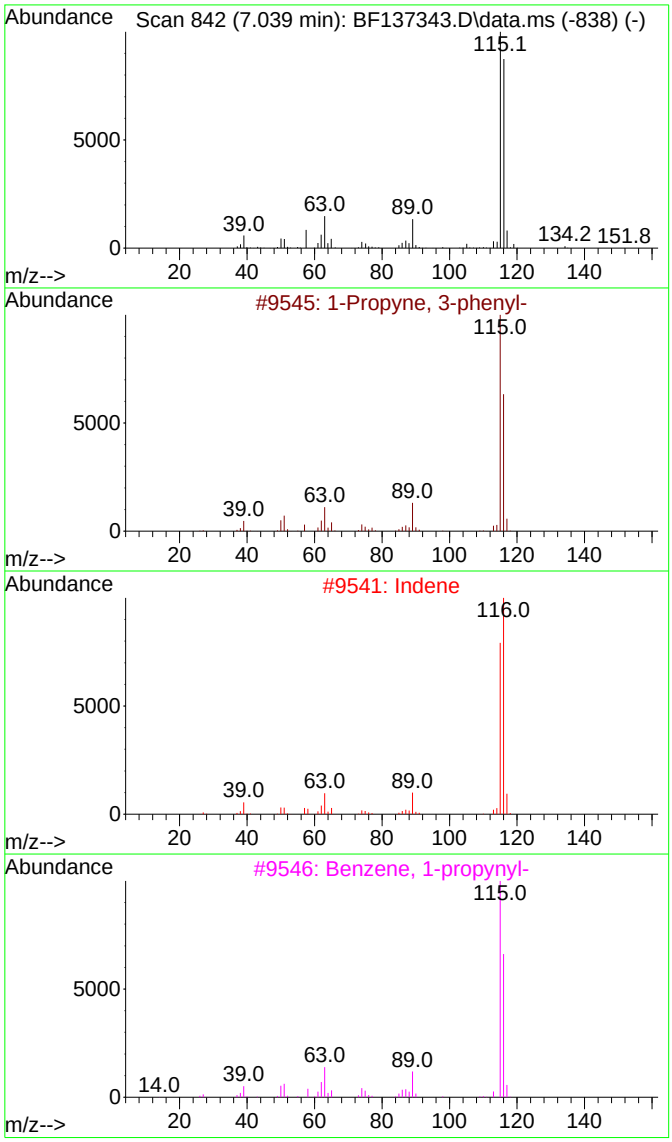
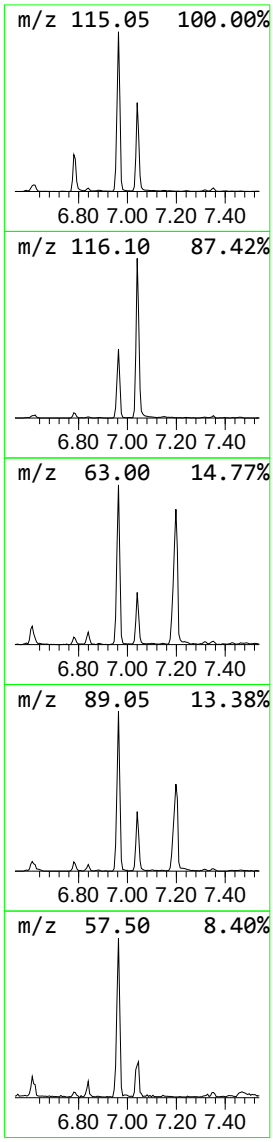
Peak Number 8 1-Propyne, 3-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.039	14.14 ng	428209	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	95
2	Indene	116	C9H8	000095-13-6	95
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	3-Methylphenylacetylene	116	C9H8	000766-82-5	91





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ALS Vial : 11 Sample Multiplier: 1

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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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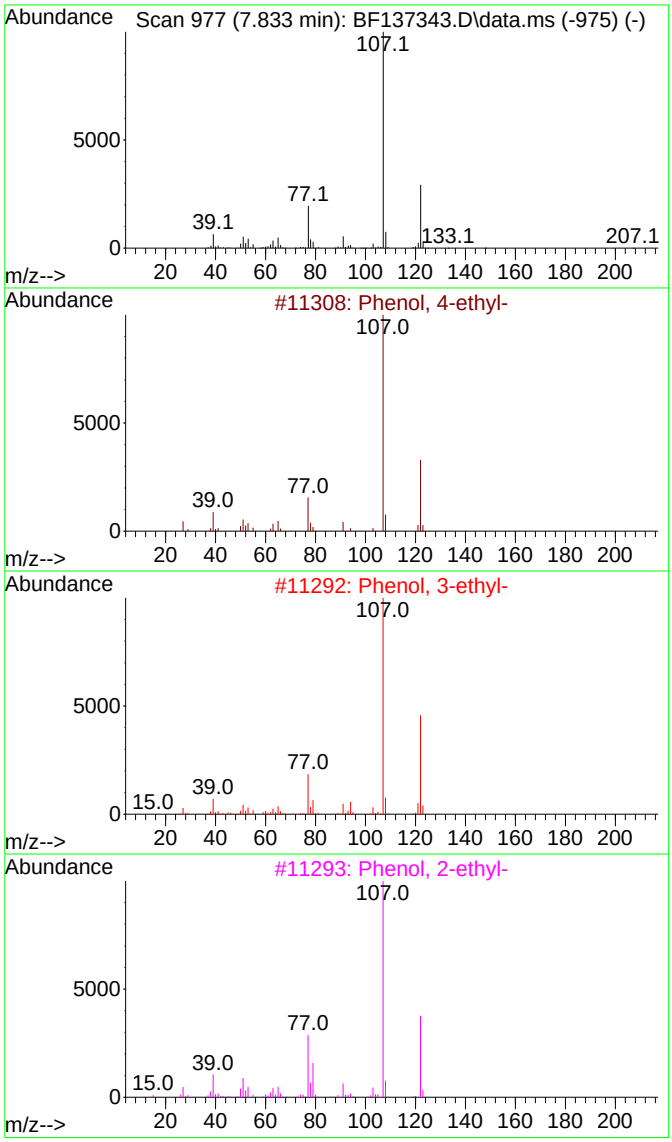
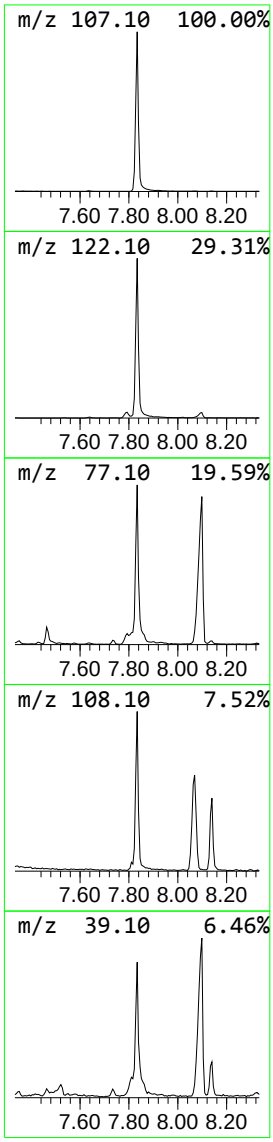
Peak Number 9 Phenol, 4-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.833	4.44 ng	2071400	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	95
2	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	86
3	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	83
4	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	72
5	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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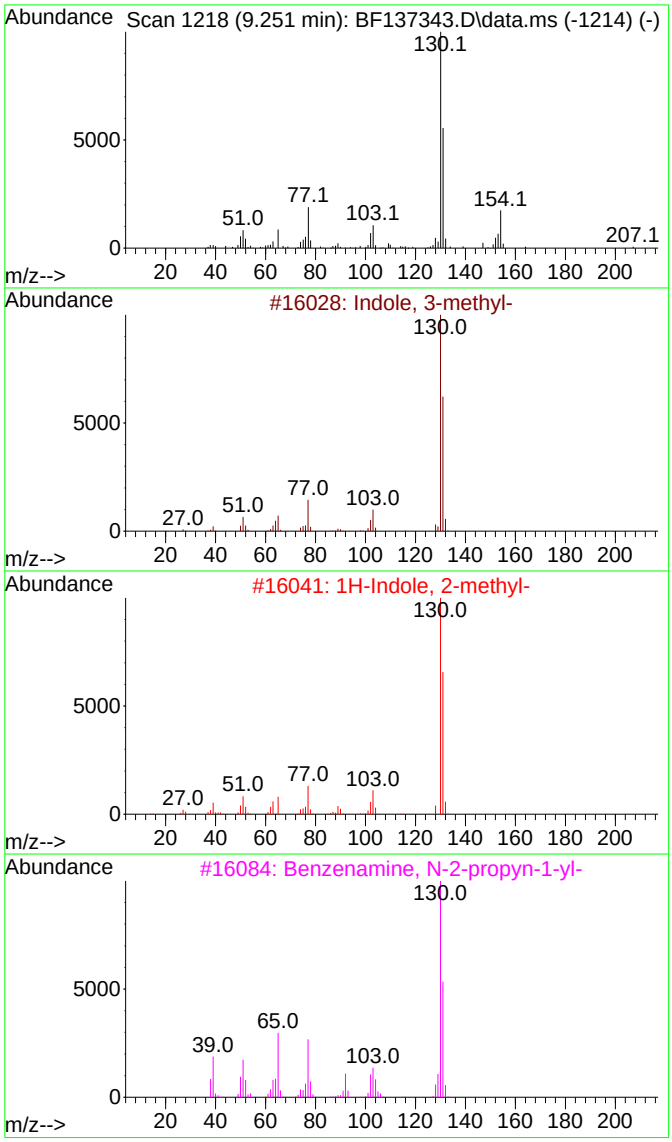
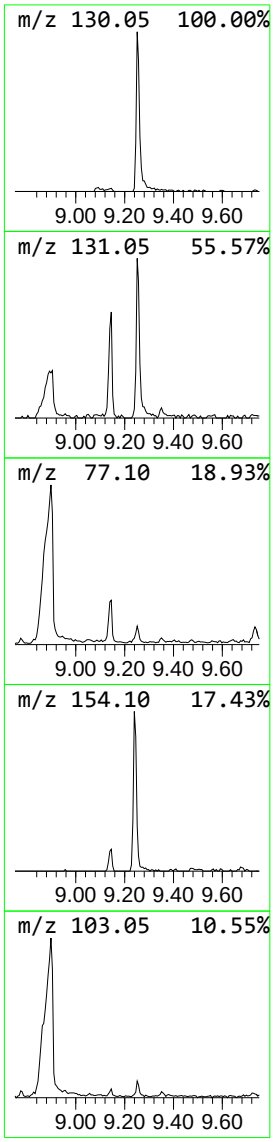
Peak Number 10 Indole, 3-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.251	2.24 ng	127262	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole, 3-methyl-	131	C9H9N	000083-34-1	87
2	1H-Indole, 2-methyl-	131	C9H9N	000095-20-5	83
3	Benzenamine, N-2-propyn-1-yl-	131	C9H9N	014465-74-8	80
4	Tryptamine	160	C10H12N2	000061-54-1	72
5	Benzonitrile, 4-formyl-	131	C8H5NO	000105-07-7	64





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Data File : BF137343.D
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Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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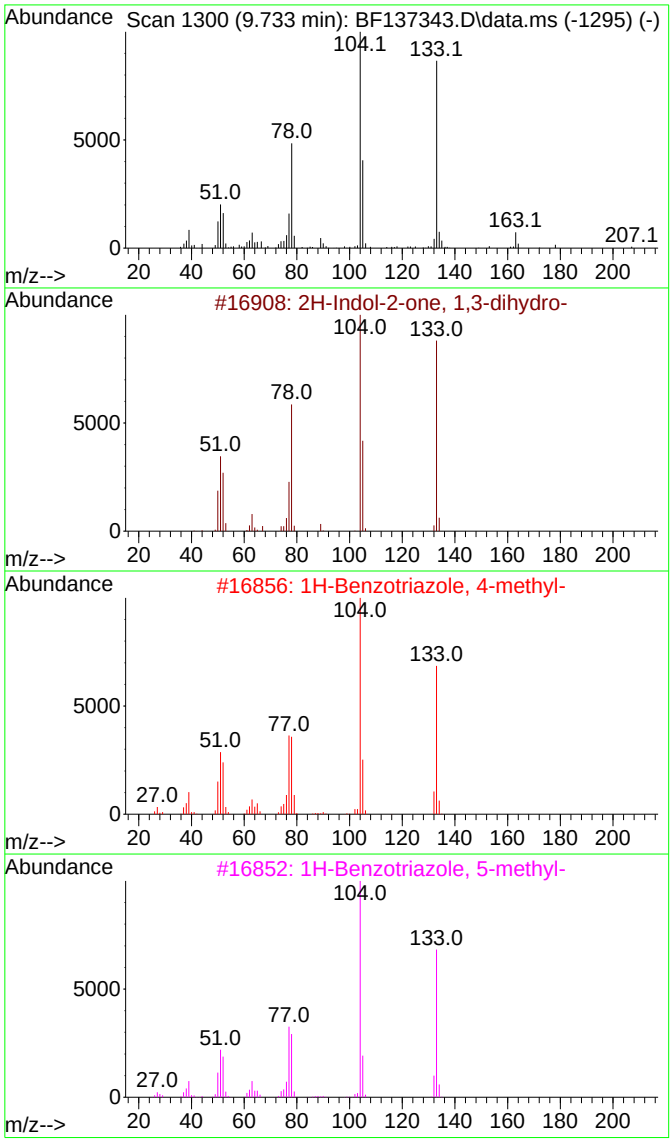
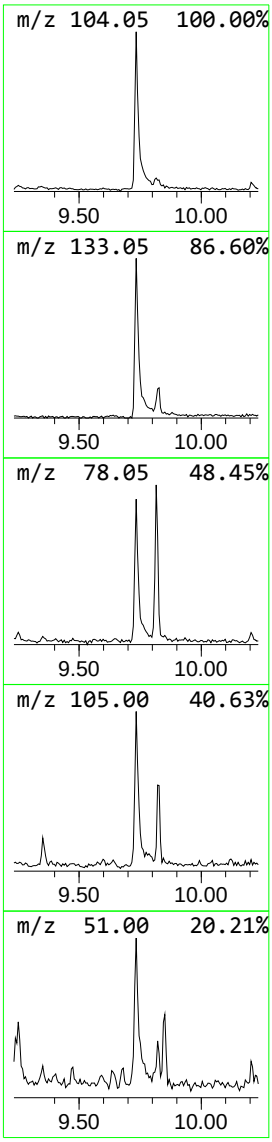
Peak Number 11 2H-Indol-2-one, 1,3-dihydro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	3.64 ng	206580	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	95
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	87
3	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	87
4	1H-Indol-5-ol	133	C8H7NO	001953-54-4	72
5	Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	72





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Data File : BF137343.D
Acq On : 08 Feb 2024 17:50
Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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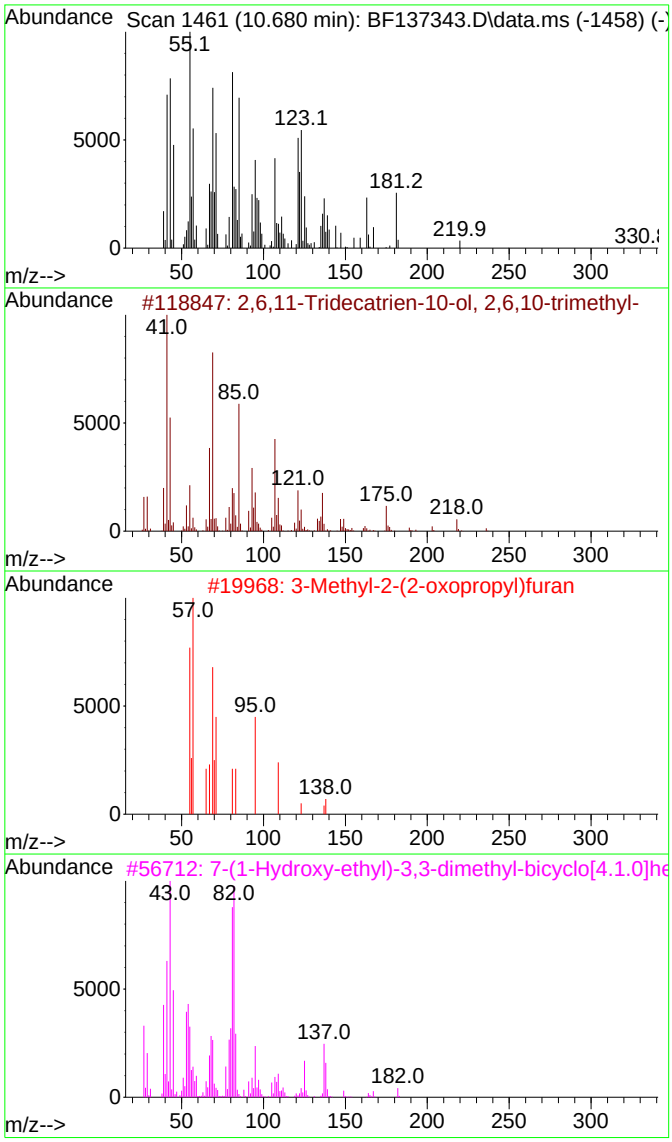
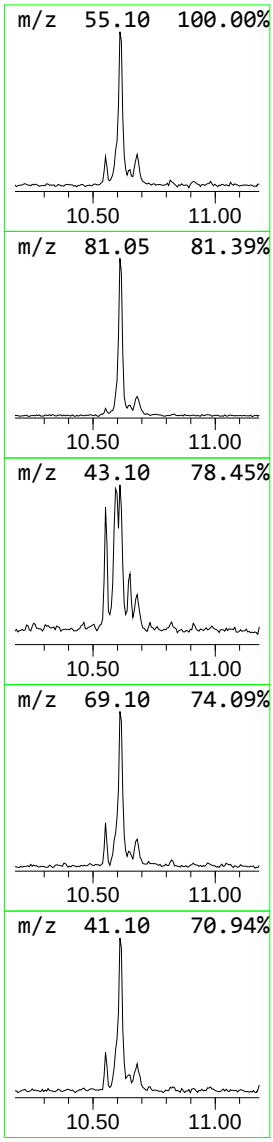
Peak Number 12 unknown10.680 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.680	3.52 ng	151569	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,11-Tridecatrien-10-ol, 2,6,1...	236	C16H28O	1000161-90-4	27
2	3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	25
3	7-(1-Hydroxy-ethyl)-3,3-dimethyl...	182	C11H18O2	1000187-18-2	20
4	Bicyclo[3.1.0]hexan-2-one, 5-(1-...	138	C9H14O	000513-20-2	18
5	9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	18





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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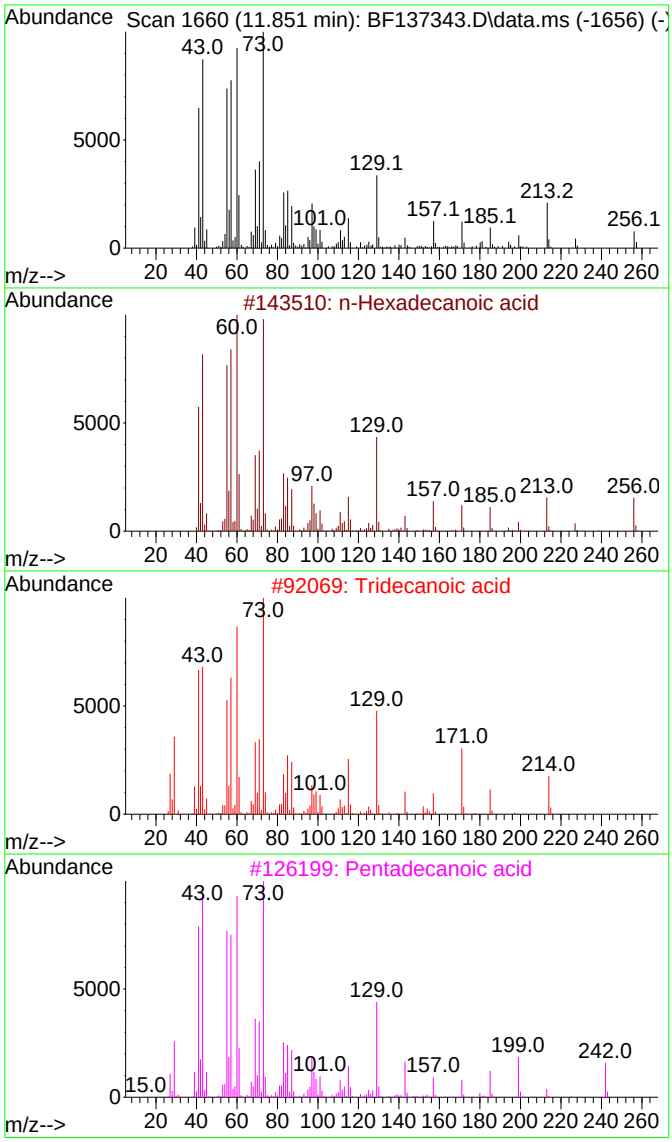
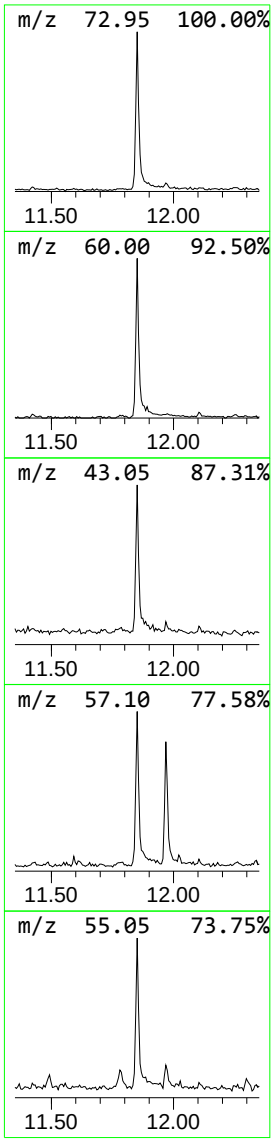
Peak Number 13 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	6.89 ng	296943	Phenanthrene-d10	11.310

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	38





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Data File : BF137343.D
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Operator : CG\JU
Sample : P1372-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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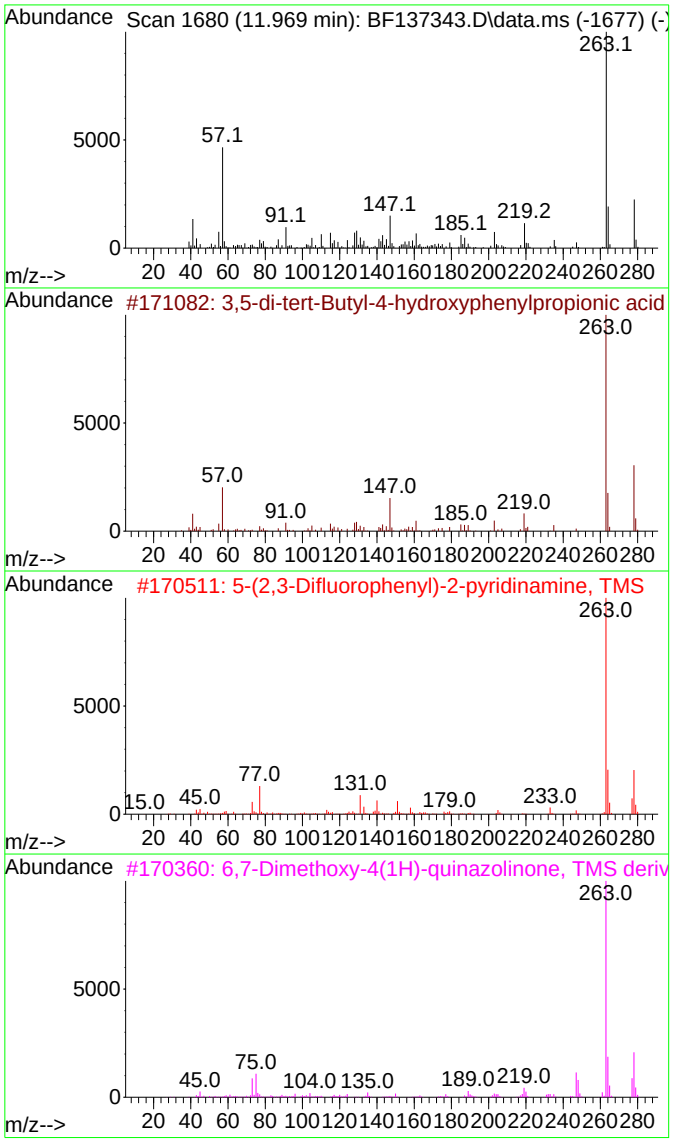
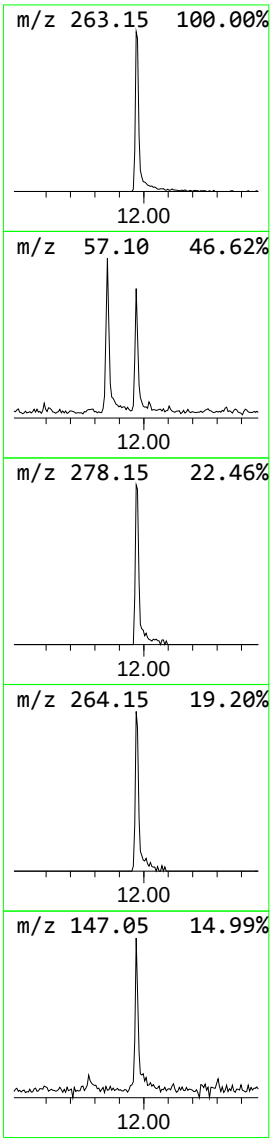
Peak Number 14 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	4.16 ng	179133	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	94
2	5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	81
3	6,7-Dimethoxy-4(1H)-quinazolinon...	278	C13H18N2O3Si	1000479-65-5	80
4	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	72
5	2,6-Bis(tert-butyl)phenol, TMS d...	278	C17H30OSi	010416-73-6	59





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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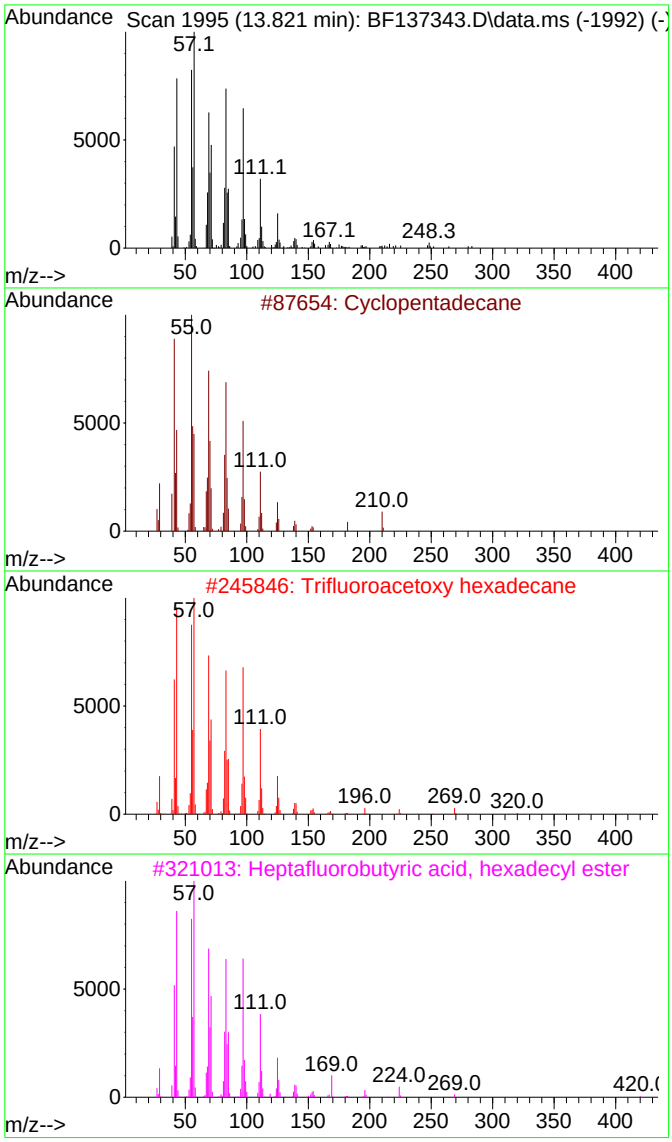
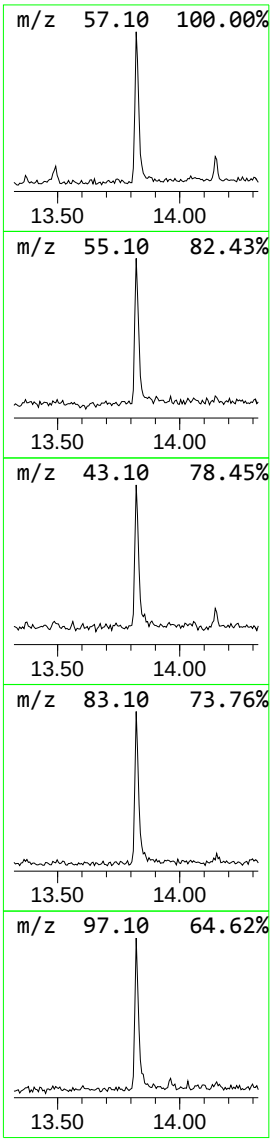
Peak Number 15 Cyclopentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	7.32 ng	215961	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137343.D
Acq On : 08 Feb 2024 17:50
Operator : CG\JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, (1-met...	5.957	13.0	ng	394600	1	6.781	605604	20.0
Benzene, 1-ethy...	6.345	5.6	ng	168721	1	6.781	605604	20.0
Benzene, 1,2,3-...	6.839	10.4	ng	315208	1	6.781	605604	20.0
Indane	6.963	70.0	ng	2119440	1	6.781	605604	20.0
1-Propyne, 3-ph...	7.039	14.1	ng	428209	1	6.781	605604	20.0
Phenol, 4-ethyl-	7.833	4.4	ng	2071400	2	8.069	9333960	20.0
Indole, 3-methyl-	9.251	2.2	ng	127262	3	9.816	1134510	20.0
2H-Indol-2-one,...	9.733	3.6	ng	206580	3	9.816	1134510	20.0
unknown10.680	10.680	3.5	ng	151569	4	11.310	861878	20.0
n-Hexadecanoic ...	11.851	6.9	ng	296943	4	11.310	861878	20.0
3,5-di-tert-But...	11.969	4.2	ng	179133	4	11.310	861878	20.0
Cyclopentadecane	13.821	7.3	ng	215961	5	13.963	589841	20.0