LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099049.D
Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.146	7	10	16	rVB	98673	125680	5.90%	0.584%
2	5.093	507	511	522	rVB	351053	406102	19.05%	1.888%
3	5.493	574	579	582	rBV	2050664	2097811	98.41%	9.751%
4	5.710	613	616	619	rBV	56080	46850	2.20%	0.218%
5	6.498	745	750	753	rBV	2146245	2048464	96.10%	9.522%
6	6.640	770	774	778	rBV	2302787	2131628	100.00%	9.908%
7	6.875	810	814	817	rBV	932067	761227	35.71%	3.538%
8	7.028	836	840	844	rBV	1860674	1643707	77.11%	7.640%
9	7.434	904	909	912	rBV	1410537	1227479	57.58%	5.706%
10	8.157	1028	1032	1035	rBV	1019301	892981	41.89%	4.151%
11	9.228	1210	1214	1217	rBV	2411629	1923337	90.23%	8.940%
12	9.616	1277	1280	1284	rBV	230870	182680	8.57%	0.849%
13	9.857	1319	1321	1326	rBV	30915	28700	1.35%	0.133%
14	9.910	1326	1330	1334	rVB	888087	735800	34.52%	3.420%
15	10.692	1460	1463	1467	rBV	835406	760934	35.70%	3.537%
16	10.804	1479	1482	1492	rVB	28101	31115	1.46%	0.145%
17	11.169	1541	1544	1547	rVB	168078	137741	6.46%	0.640%
18	11.392	1579	1582	1586	rBV	689603	604646	28.37%	2.810%
19	12.974	1847	1851	1855	rBV	1660081	1472359	69.07%	6.844%
20	13.833	1993	1997	2000	rBV	422621	338551	15.88%	1.574%
21	13.863	2000	2002	2013	rVB	105763	116562	5.47%	0.542%
22	14.033	2027	2031	2035	rBV	853884	735354	34.50%	3.418%
23	14.163	2050	2053	2056	rBV	599403	509201	23.89%	2.367%
24	14.204	2056	2060	2062	rVV	904276	773790	36.30%	3.597%
25	14.227	2062	2064	2066	rVV	279788	251063	11.78%	1.167%
26	14.251	2066	2068	2071	rVB	351551	286512	13.44%	1.332%
27	14.498	2105	2110	2115	rBV	44548	68938	3.23%	0.320%
28	14.545	2115	2118	2122	rVB	154558	134528	6.31%	0.625%
29	14.615	2127	2130	2133	rVB	51323	46717	2.19%	0.217%
30	15.133	2215	2218	2222	rBV	37497	39832	1.87%	0.185%
31	15.510	2276	2282	2289	rBV	632686	799139	37.49%	3.715%
32	15.951	2354	2357	2362	rVB	43106	59274	2.78%	0.276%
33	16.462	2440	2444	2450	rVB2	28189	45066	2.11%	0.209%
34	17.568	2628	2632	2641	rVB2	22459	50167	2.35%	0.233%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099049.D
Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 21513935

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099049.D
Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
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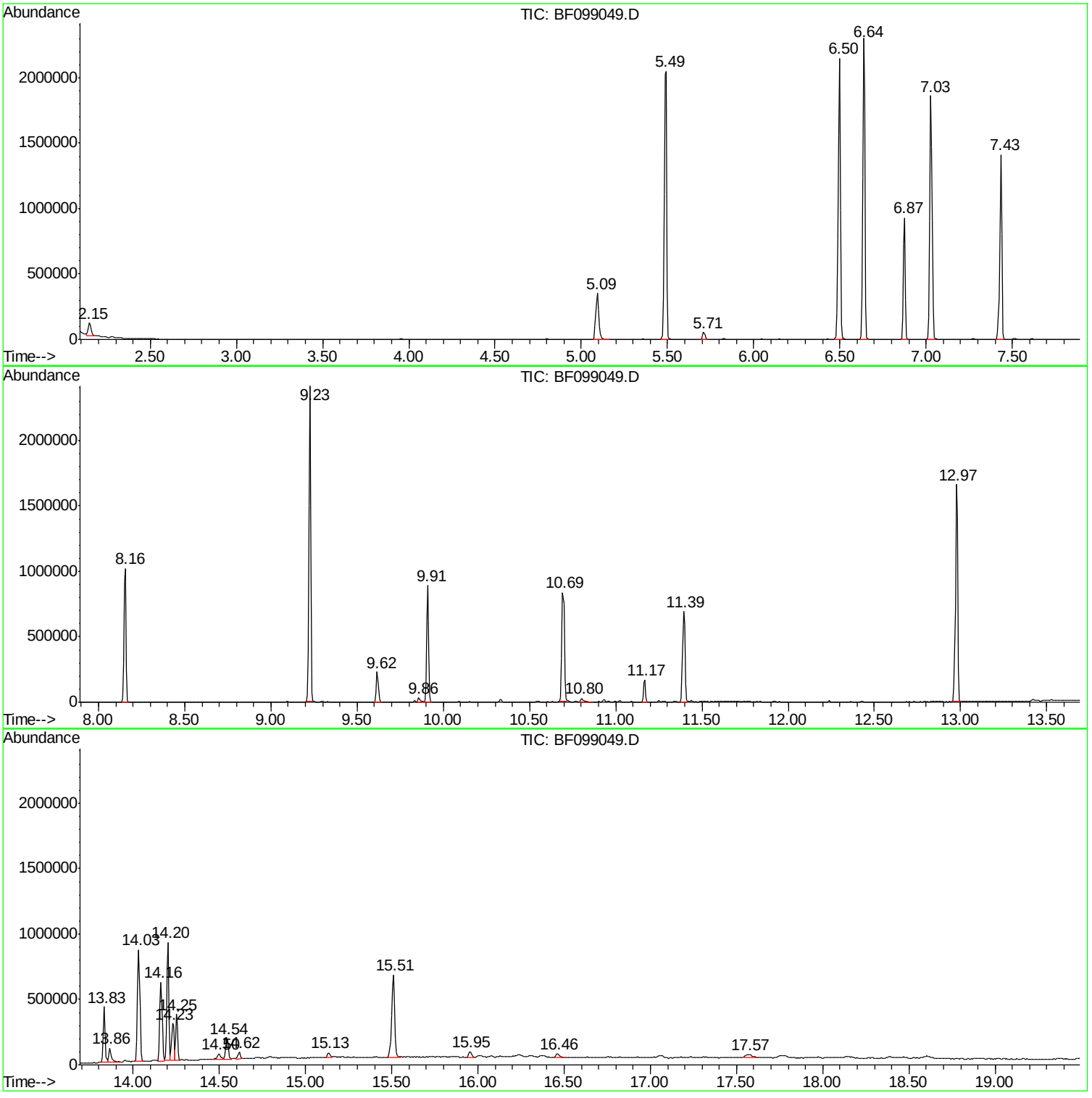
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Acq On : 4 Oct 2017 00:02
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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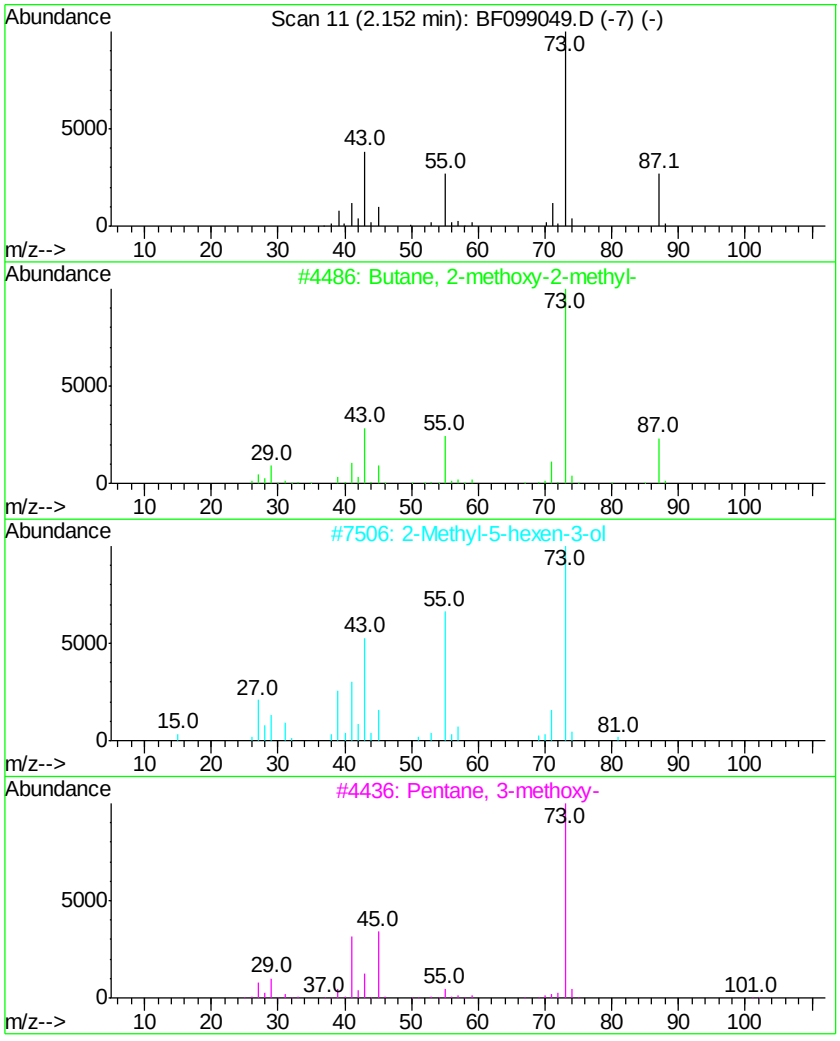
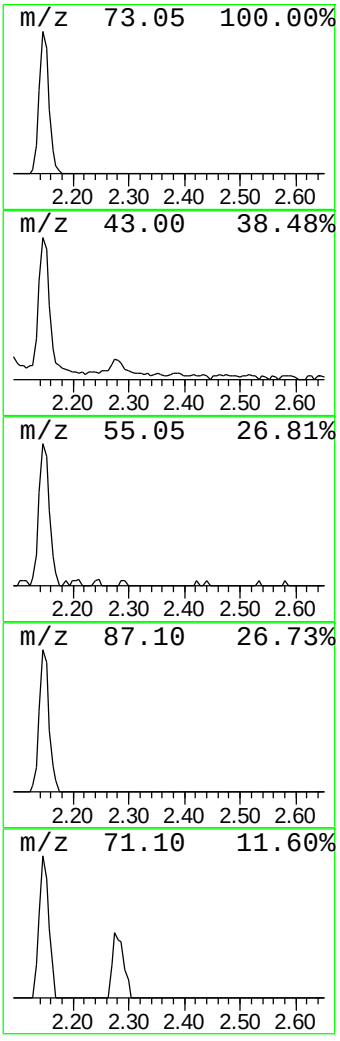
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	3.30 ng	125680	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	10





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Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

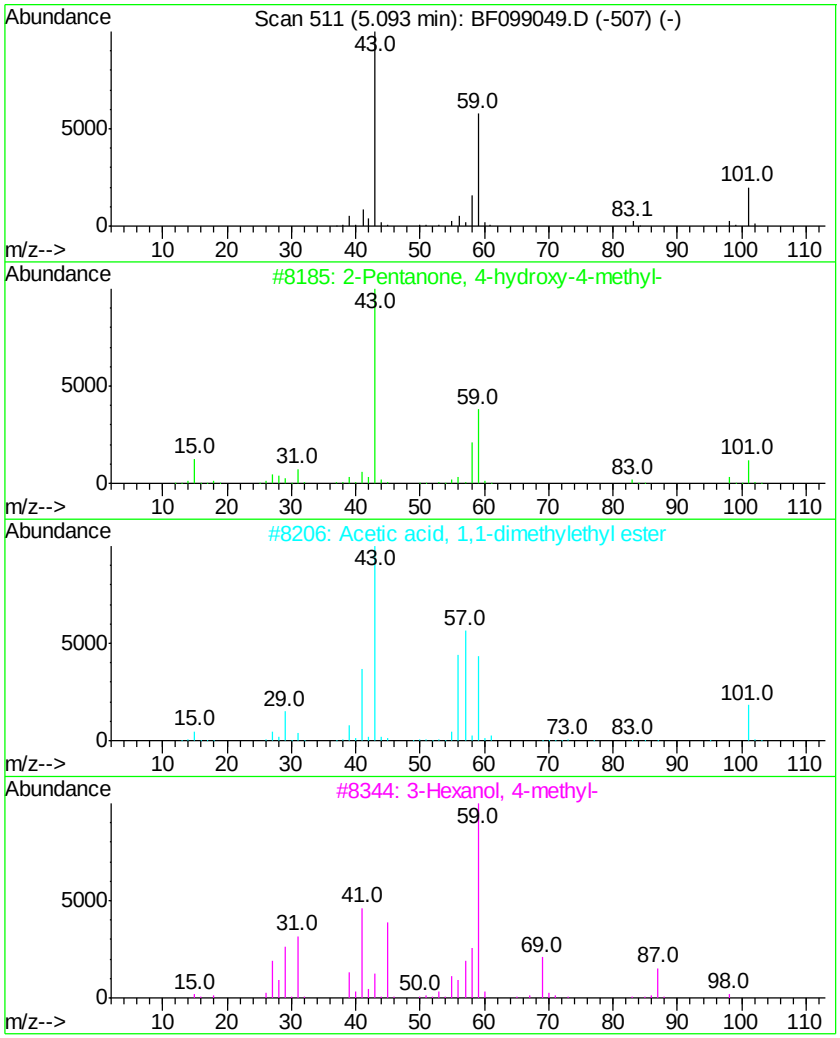
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

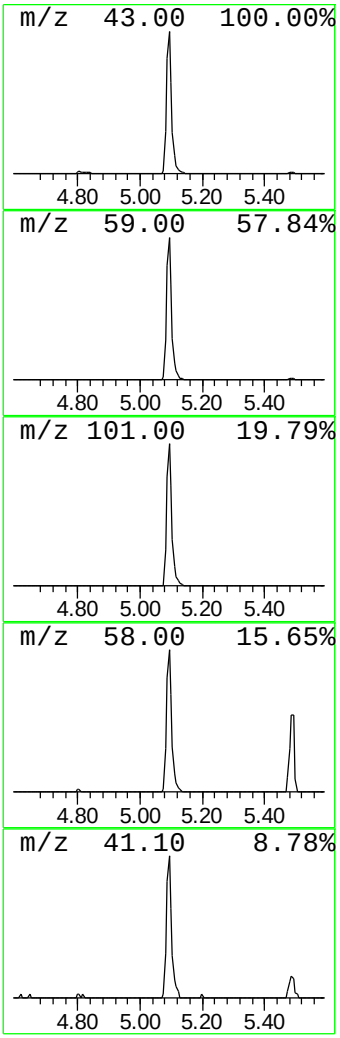
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	10.67 ng	406102	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

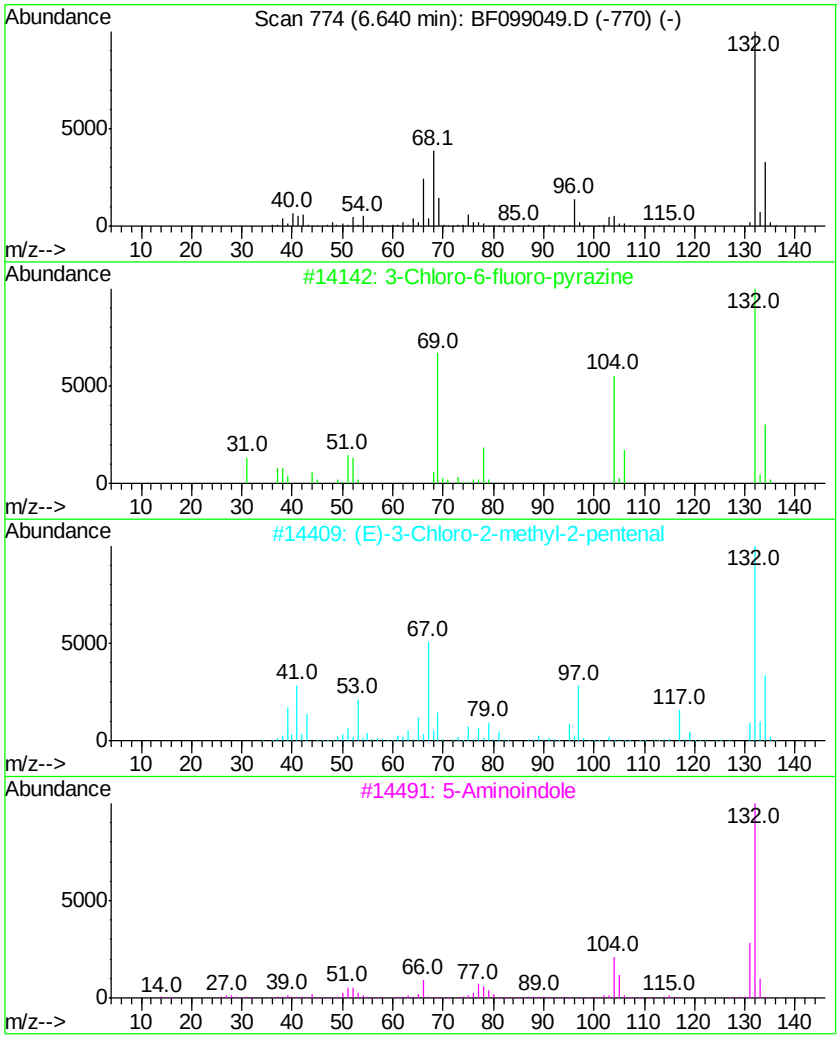
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

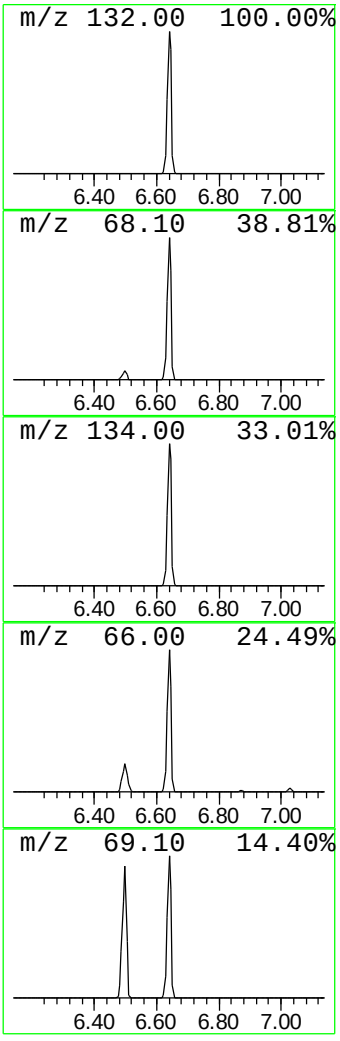
****

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	56.01 ng	2131630	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

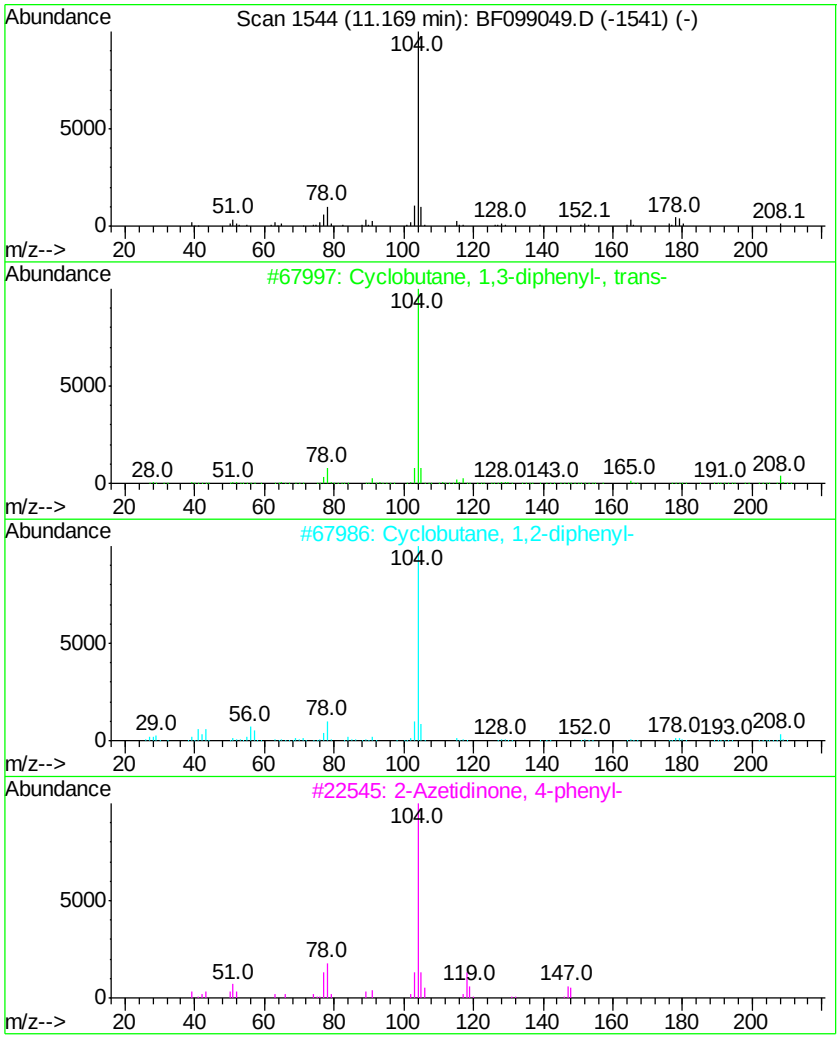
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

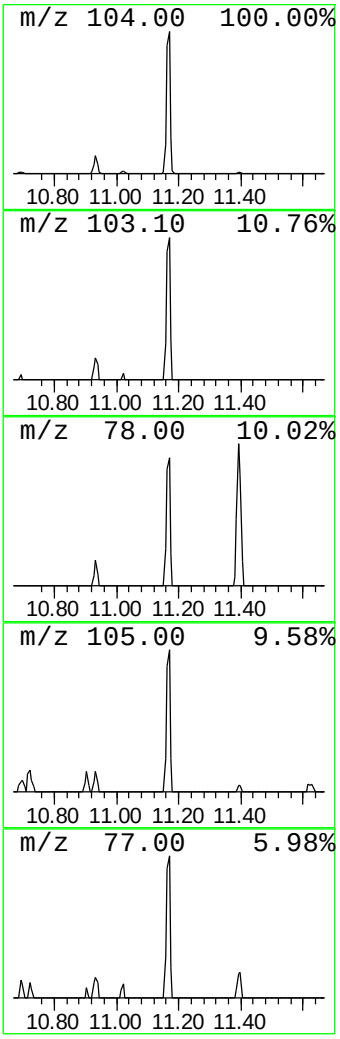
****

Peak Number 5 Cyclobutane, 1,3-diphenyl-,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	4.56 ng	137741	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, 1,3-diphenyl-, trans-	208	C16H16	025558-23-0	72
2	Cyclobutane, 1,2-diphenyl-	208	C16H16	003018-21-1	56
3	2-Azetidinone, 4-phenyl-	147	C9H9NO	005661-55-2	56
4	2-Furanone, 4-phenyltetrahydro	162	C10H10O2	1000197-38-4	56
5	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	49





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Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

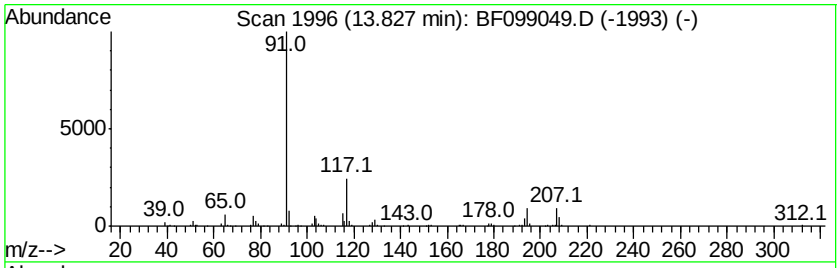
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

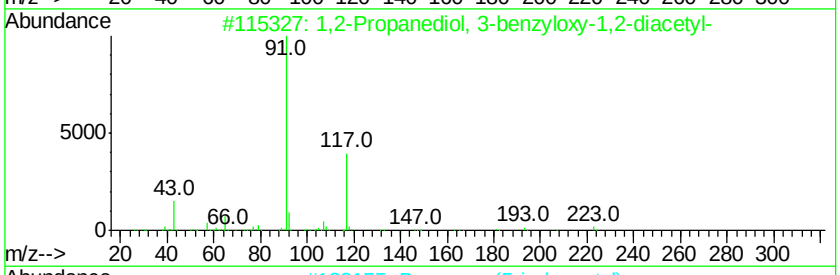
****

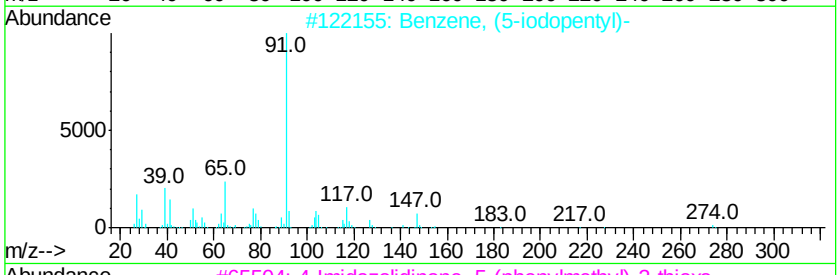
Peak Number 6 unknown13.83 Concentration Rank 6

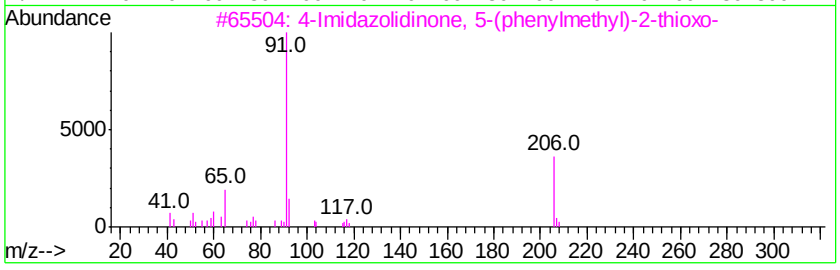
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	9.21 ng	338551	Chrysene-d12	14.03

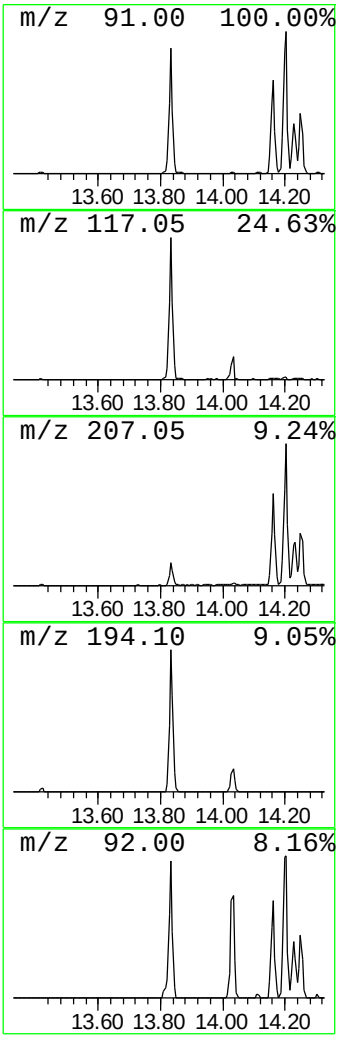
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Propanediol, 3-benzyloxy-1,2...	266	C14H18O5	013754-10-4	32
2	Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
3	4-Imidazolidinone, 5-(phenylmeth...	206	C10H10N2OS	006330-09-2	17
4	Isoxazole, 5-chloro-4-(2-phenyle...	207	C11H10ClNO	1000362-09-0	16
5	Alpha-phenyl-alpha-tropylacetald...	378	C22H22N2O2S	022532-16-7	12











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Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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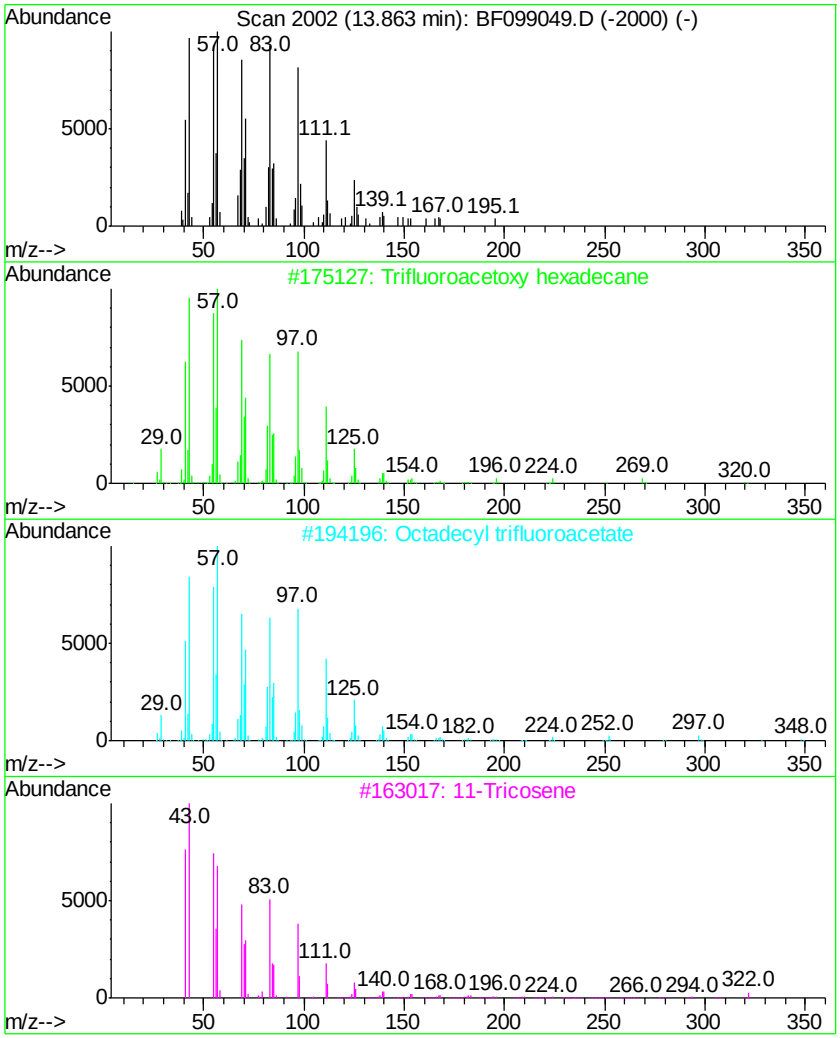
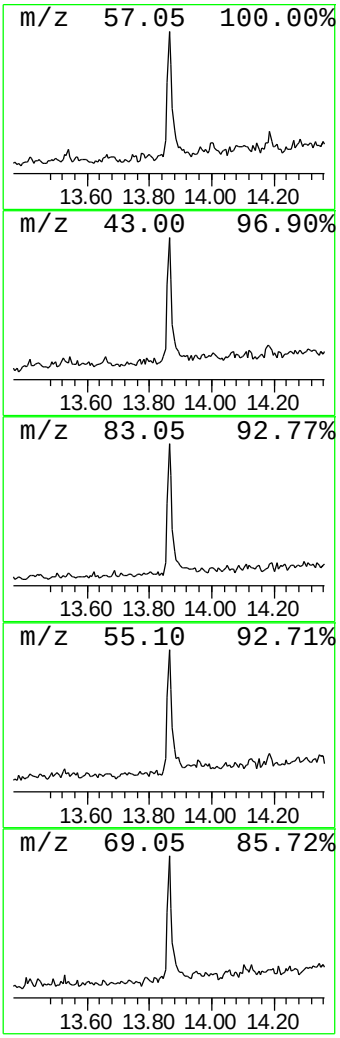
Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.17 ng	116562	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92
3	11-Tricosene	322	C23H46	052078-56-5	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	81





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TIC Library : C:\DATABASE\NIST11.L
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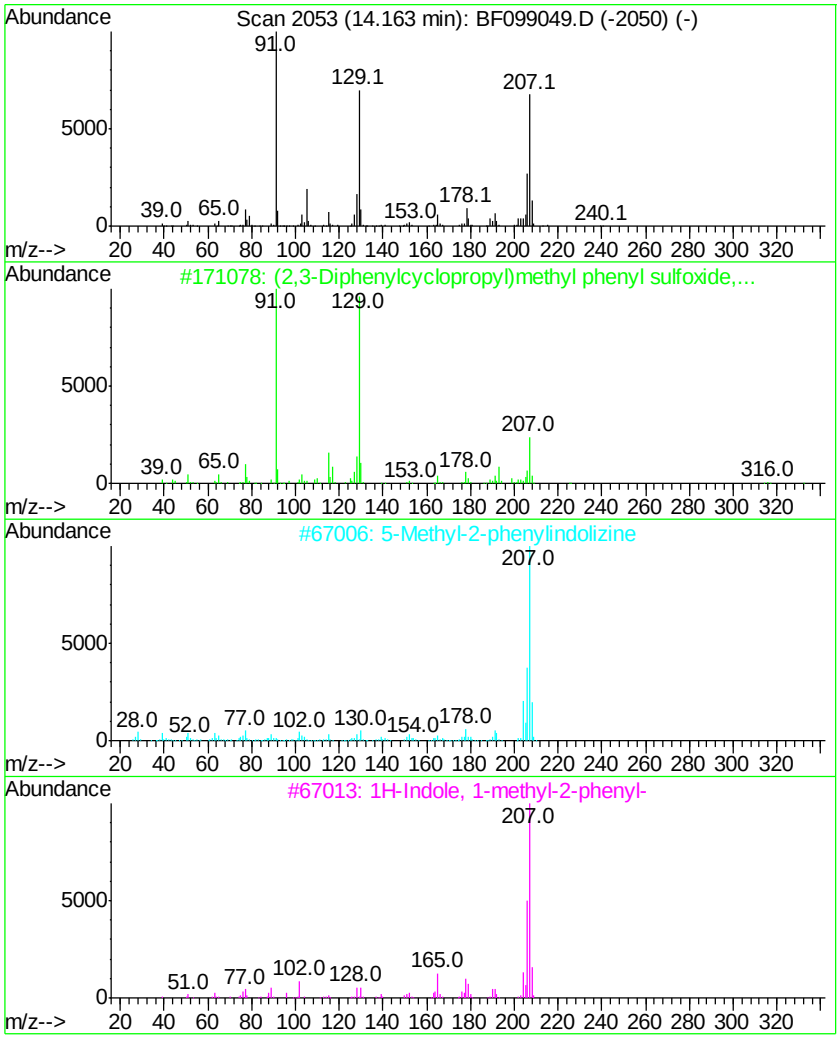
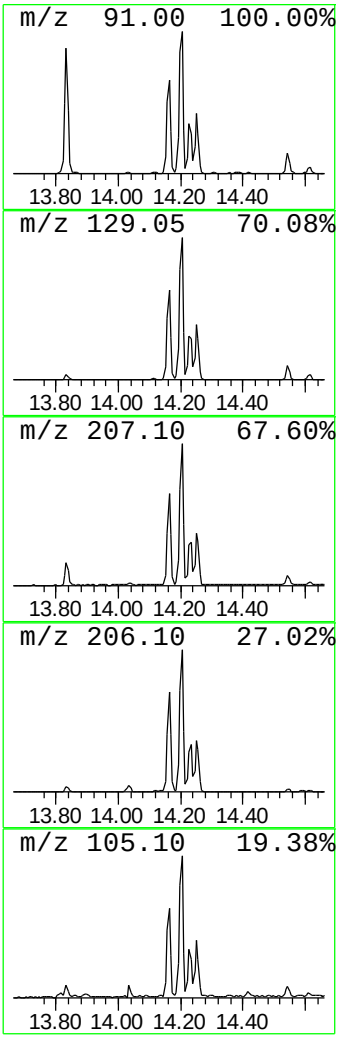
Peak Number 8 unknown14.16 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	13.85 ng	509201	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	42
2	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
4	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38
5	Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	37





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Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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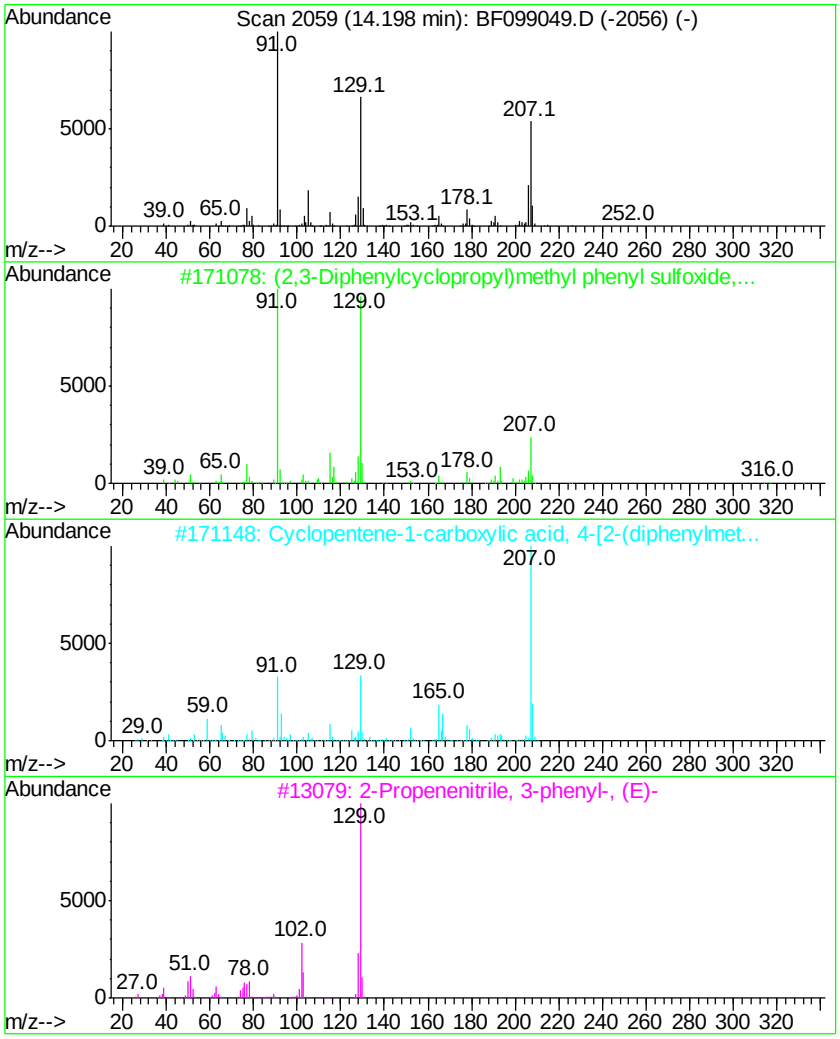
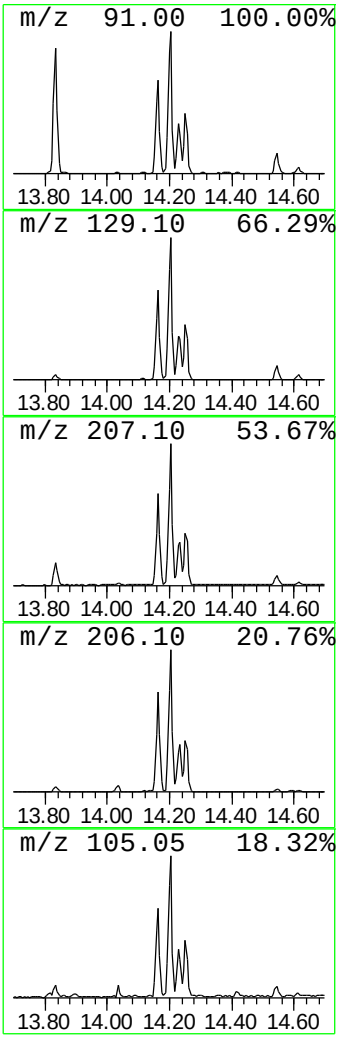
Peak Number 9 unknown14.20 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	21.05 ng	773790	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	43
2	Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	40
3	2-Propenenitrile, 3-phenyl-, (E)-	129	C9H7N	001885-38-7	27
4	Quinoline	129	C9H7N	000091-22-5	27
5	Isoquinoline	129	C9H7N	000119-65-3	27





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Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

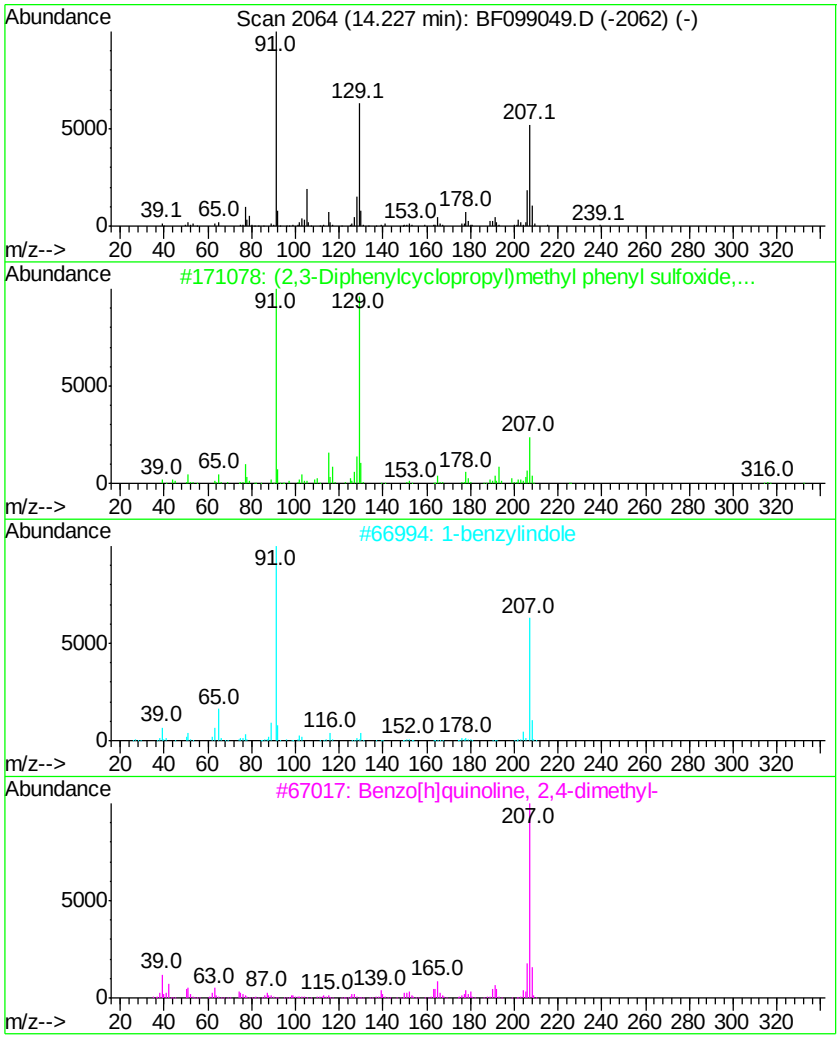
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

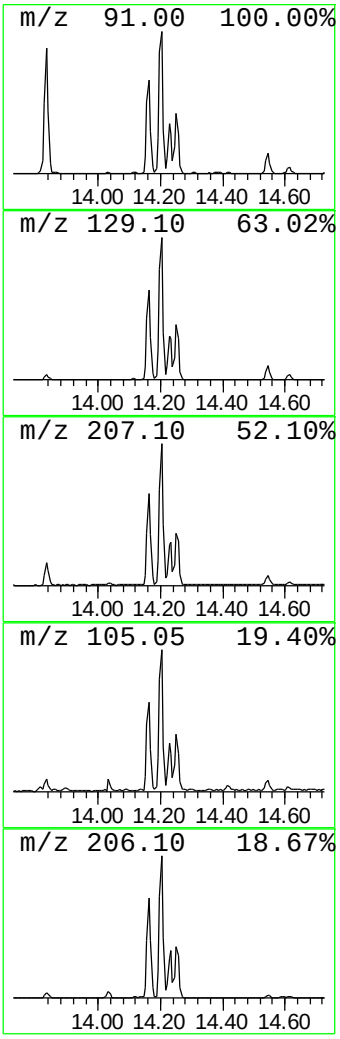
****

Peak Number 10 unknown14.23 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	6.83 ng	251063	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	38
2	1-benzylindole	207	C15H13N	1000334-31-3	35
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	30
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	30
5	6-Methyl-5-[1-piperidinyl]-2,4-p...	207	C10H17N5	164589-37-1	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099049.D
Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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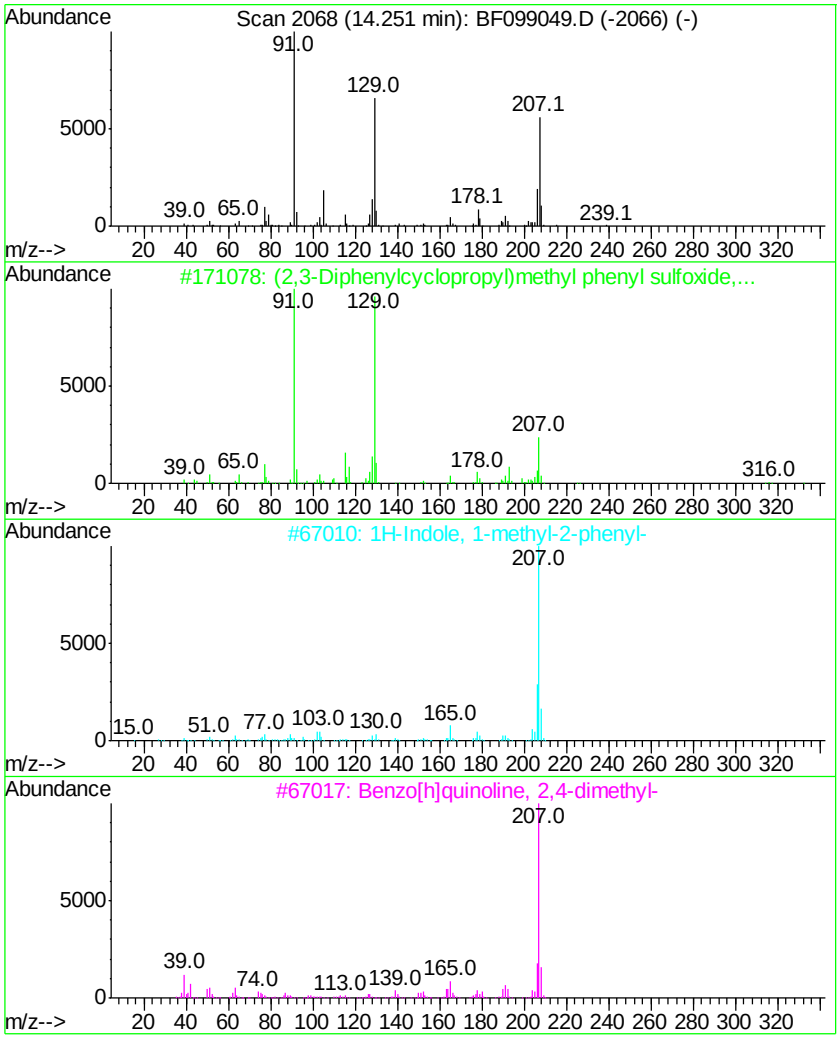
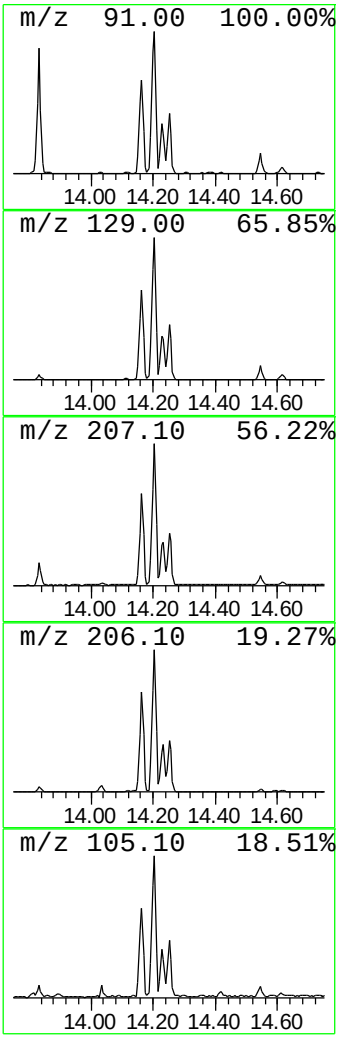
Peak Number 11 (2,3-Diphenylcyclopropyl)me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	7.79 ng	286512	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	78
2	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	35
4	1-benzylindole	207	C15H13N	1000334-31-3	35
5	Phenanthridinium, 5,6-dimethyl-,...	335	C15H14IN	016511-48-1	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099049.D
Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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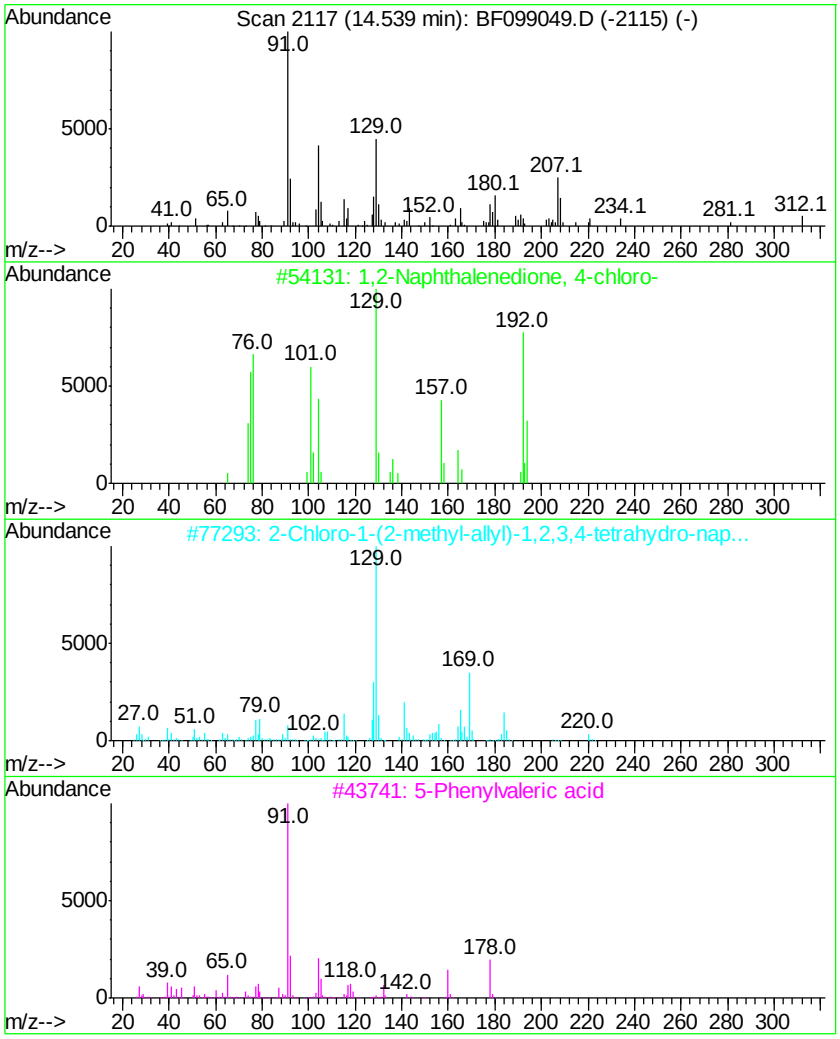
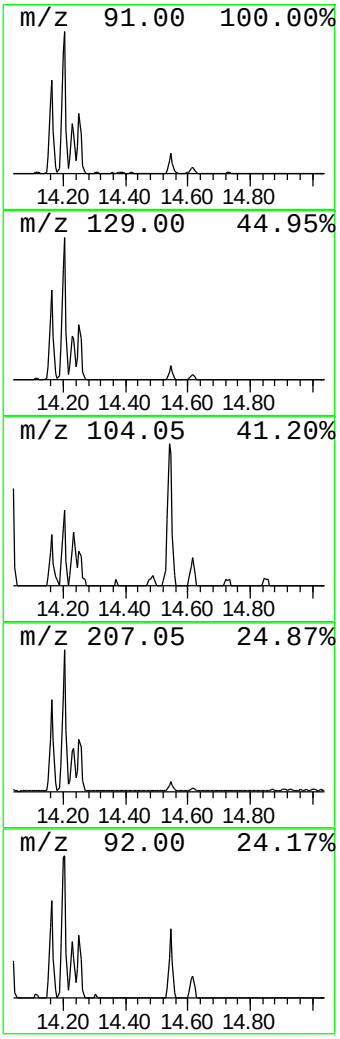
Peak Number 12 unknown14.54 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.66 ng	134528	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Naphthalenedione, 4-chloro-	192	C10H5ClO2	006655-90-9	22
2	2-Chloro-1-(2-methyl-allyl)-1,2,...	220	C14H17Cl	1000185-82-6	11
3	5-Phenylvaleric acid	178	C11H14O2	002270-20-4	10
4	3,6-Dibromo-1a,2,2a,3,6,6a,7,7a-...	306	C10H12Br2O	1000188-45-5	10
5	2-Hexenal, 6-phenyl-, (E)-	174	C12H14O	055282-87-6	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099049.D
Acq On : 4 Oct 2017 00:02
Operator : SJ/JU
Sample : I5598-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.15	3.3	ng	125680	1	6.87	761227	20.0
2-Pentanone, 4-hy...	5.09	10.7	ng	406102	1	6.87	761227	20.0
unknown6.64	6.64	56.0	ng	2131630	1	6.87	761227	20.0
Cyclobutane, 1,3-...	11.17	4.6	ng	137741	4	11.39	604646	20.0
unknown13.83	13.83	9.2	ng	338551	5	14.03	735354	20.0
Trifluoroacetoxy ...	13.86	3.2	ng	116562	5	14.03	735354	20.0
unknown14.16	14.16	13.9	ng	509201	5	14.03	735354	20.0
unknown14.20	14.20	21.1	ng	773790	5	14.03	735354	20.0
unknown14.23	14.23	6.8	ng	251063	5	14.03	735354	20.0
(2,3-Diphenylcycl...	14.25	7.8	ng	286512	5	14.03	735354	20.0
unknown14.54	14.54	3.7	ng	134528	5	14.03	735354	20.0