LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137344.D
Acq On : 08 Feb 2024 18:19
Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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: BF137344.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	546	rBV	3159547	2918203	21.67%	5.836%
2	5.416	558	566	573	rBV2	1616293	1825446	13.55%	3.651%
3	5.640	600	604	608	rBV	545353	497126	3.69%	0.994%
4	6.416	733	736	742	rBV2	958973	1149681	8.54%	2.299%
5	6.469	742	745	749	rVB	249600	210592	1.56%	0.421%
6	6.610	766	769	775	rVB2	248332	254922	1.89%	0.510%
7	6.781	795	798	803	rBV	634174	595672	4.42%	1.191%
8	6.839	805	808	814	rVB	200759	173080	1.29%	0.346%
9	6.963	825	829	832	rBV	1506472	1240192	9.21%	2.480%
10	7.039	838	842	851	rVB	396107	347864	2.58%	0.696%
11	7.222	863	873	876	rBV	6929598	13467878	100.00%	26.934%
12	7.351	887	895	903	rBV	1849278	2119922	15.74%	4.240%
13	7.545	920	928	932	rVB	161335	315575	2.34%	0.631%
14	7.834	974	977	986	rVB2	739590	1252636	9.30%	2.505%
15	8.092	1012	1021	1024	rBV2	4983885	5752002	42.71%	11.503%
16	8.133	1025	1028	1035	rVB	716310	648974	4.82%	1.298%
17	8.339	1057	1063	1068	rBV	219319	339715	2.52%	0.679%
18	8.875	1147	1154	1156	rBV2	913754	1386669	10.30%	2.773%
19	8.910	1156	1160	1163	rVB	1042720	1546063	11.48%	3.092%
20	9.145	1195	1200	1203	rVV	3467597	3326321	24.70%	6.652%
21	9.639	1280	1284	1288	rBV2	140055	186899	1.39%	0.374%
22	9.733	1296	1300	1306	rBV2	161820	263643	1.96%	0.527%
23	9.822	1311	1315	1318	rVV2	1165235	1252926	9.30%	2.506%
24	10.551	1436	1439	1442	rVV	379265	307380	2.28%	0.615%
25	10.610	1442	1449	1454	rVV2	2485761	2675112	19.86%	5.350%
26	10.727	1466	1469	1478	rVB2	129511	160586	1.19%	0.321%
27	11.310	1564	1568	1576	rBV	943894	791544	5.88%	1.583%
28	11.851	1657	1660	1667	rBV	470503	469127	3.48%	0.938%
29	11.974	1678	1681	1688	rBV	524738	490731	3.64%	0.981%
30	12.639	1791	1794	1801	rBV	151915	160921	1.19%	0.322%
31	12.910	1836	1840	1843	rBV	2780178	2436322	18.09%	4.872%
32	13.821	1992	1995	2005	rVB	227430	254754	1.89%	0.509%
33	13.963	2016	2019	2025	rVB	633552	538533	4.00%	1.077%
34	15.445	2266	2271	2280	rVB	527227	646809	4.80%	1.294%

Sum of corrected areas: 50003820

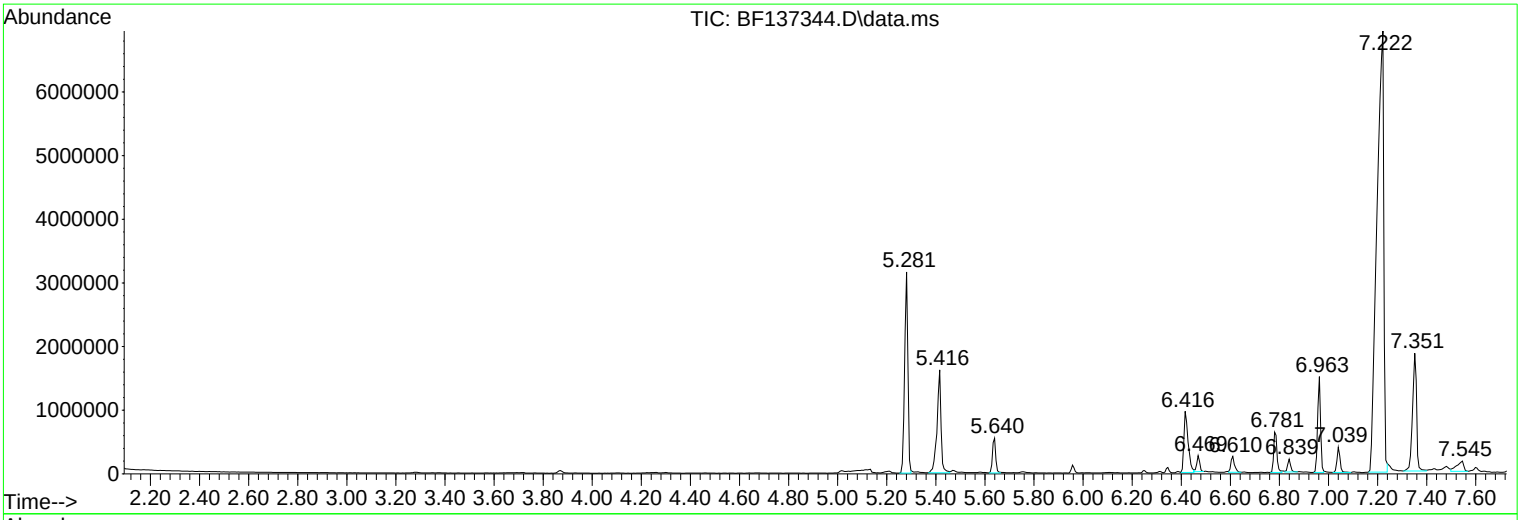
Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

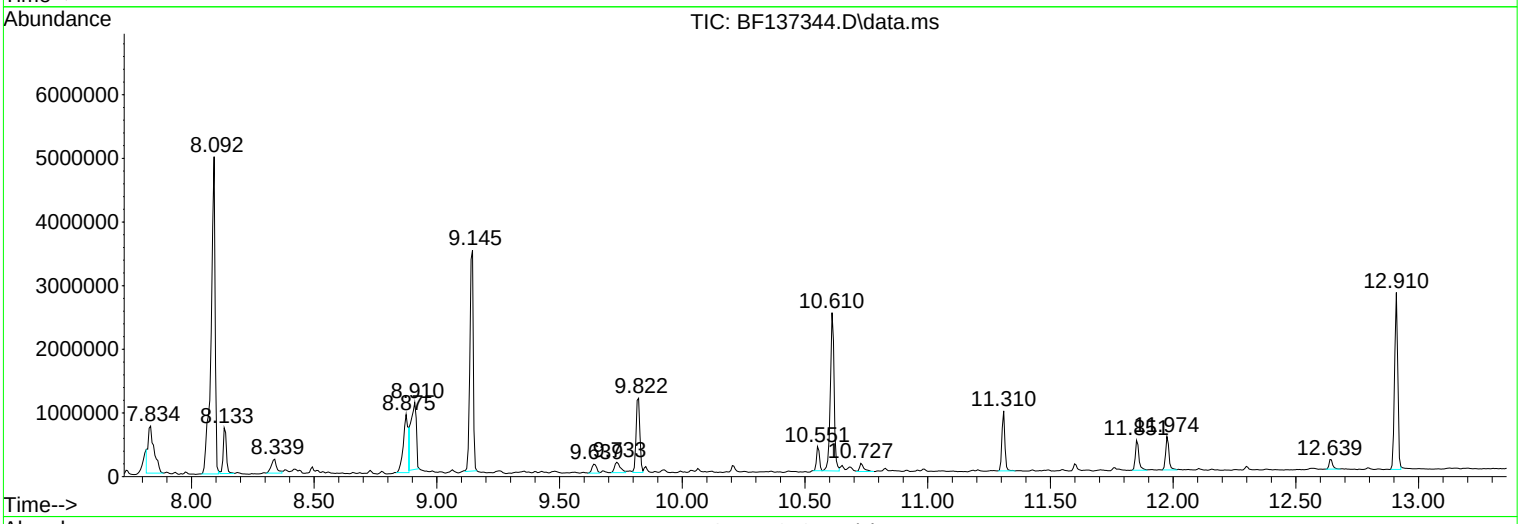
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137344.D
Acq On : 08 Feb 2024 18:19
Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

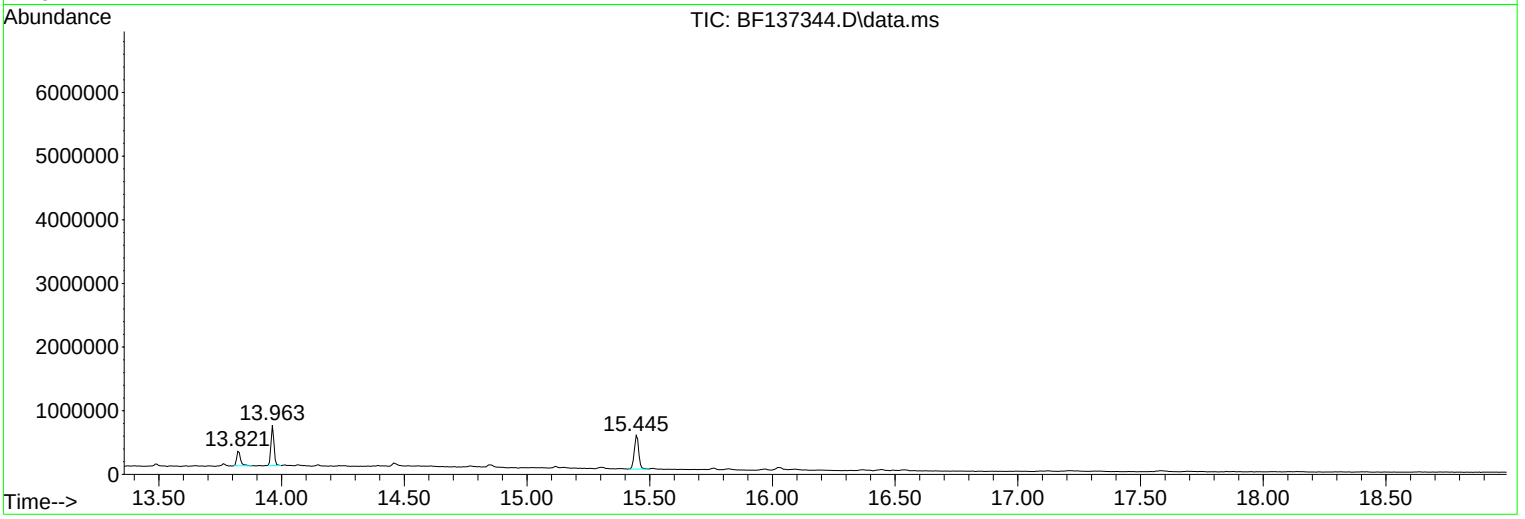
Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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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TIC Library : C:\Database\NIST20.L
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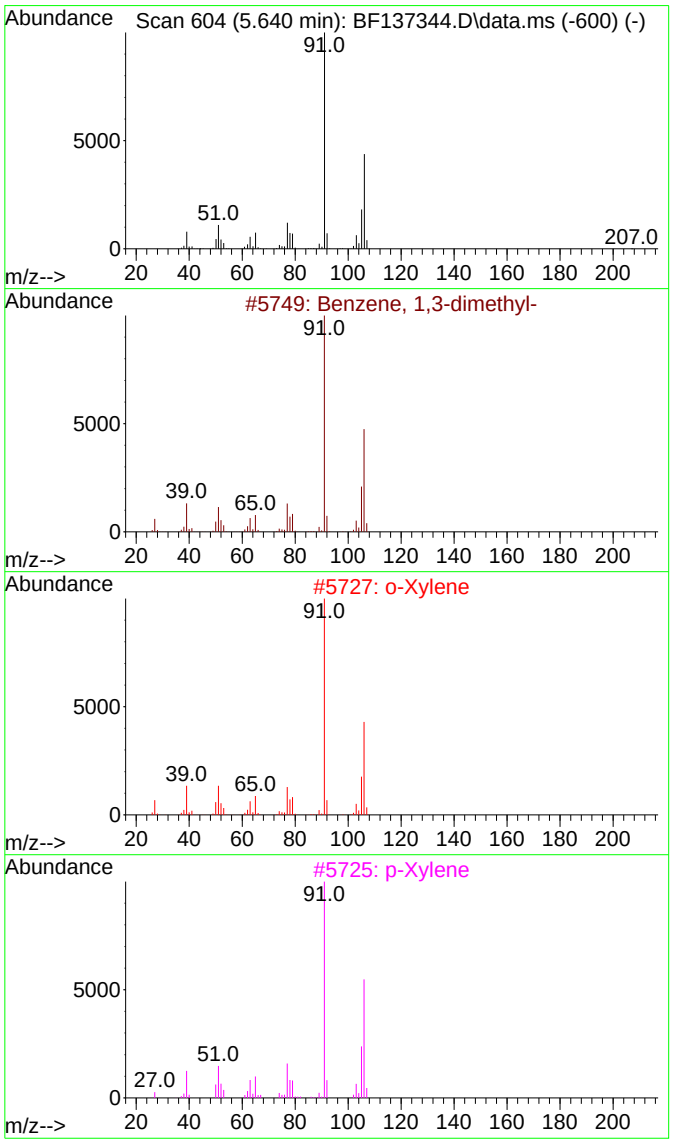
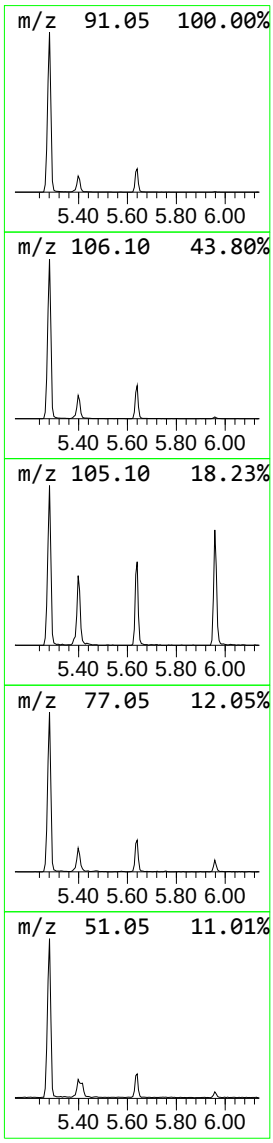
****

Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.640	16.69 ng	497126	1,4-Dichlorobenzene-d4	6.787

Hit# of 4	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2	o-Xylene	106	C8H10	000095-47-6	97
3	p-Xylene	106	C8H10	000106-42-3	97
4	Ethylbenzene	106	C8H10	000100-41-4	91





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Acq On : 08 Feb 2024 18:19
Operator : CG\JU
Sample : P1372-08
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
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TIC Library : C:\Database\NIST20.L
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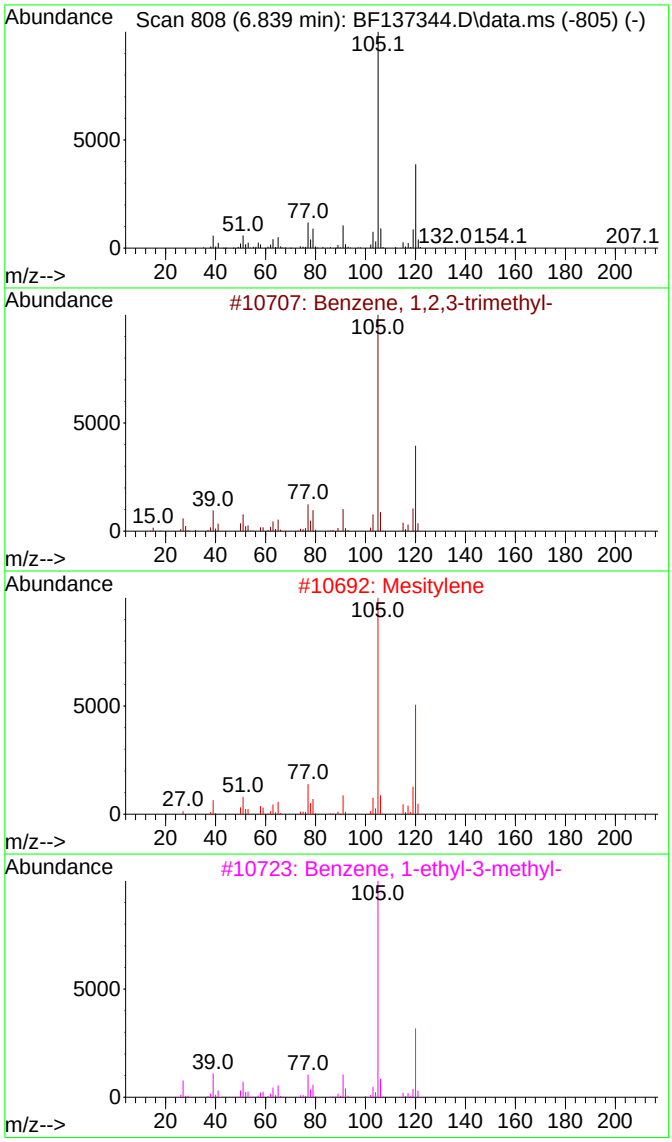
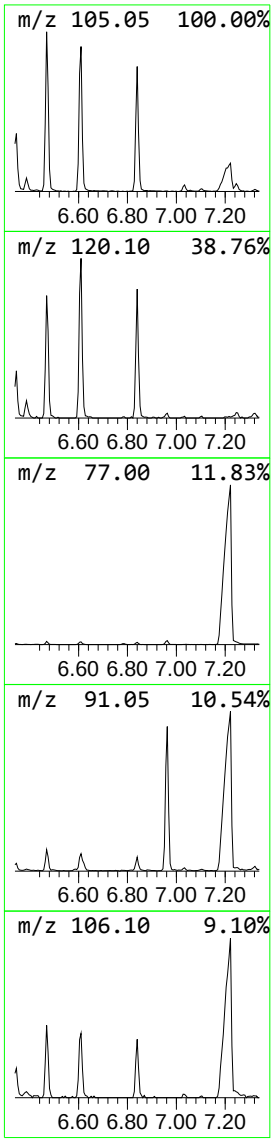
Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.839	5.81 ng	173080	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Data File : BF137344.D
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Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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

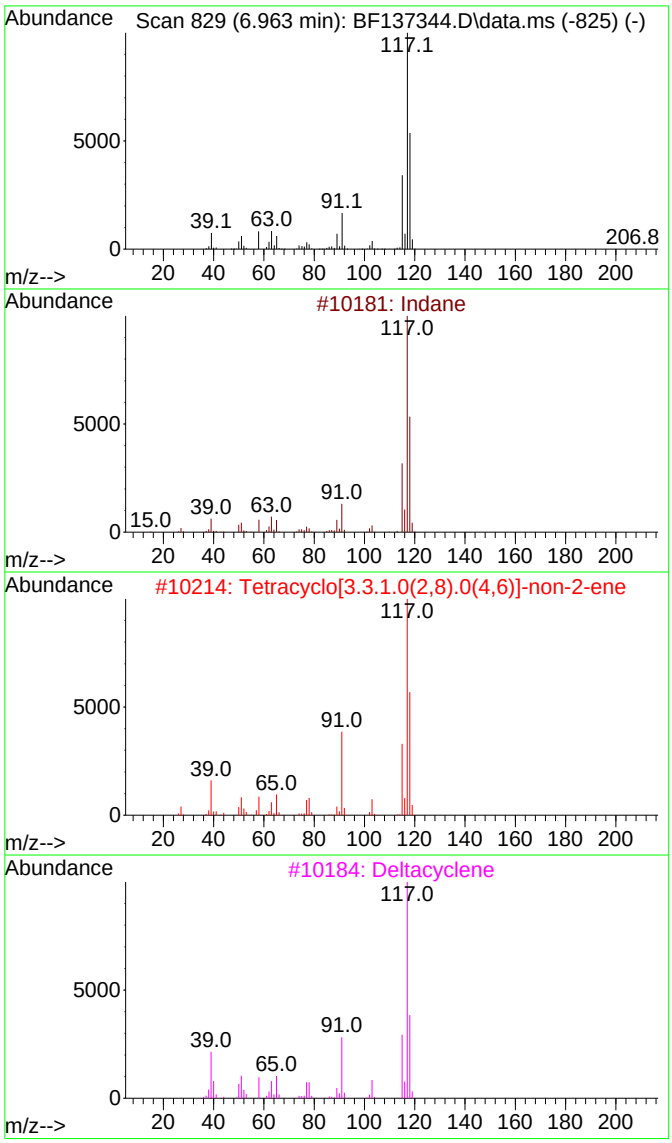
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

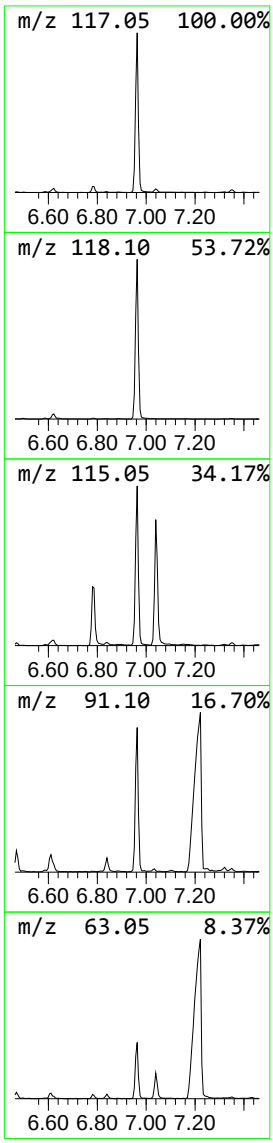
****

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	41.64 ng	1240190	1,4-Dichlorobenzene-d4	6.787

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	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	53





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Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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

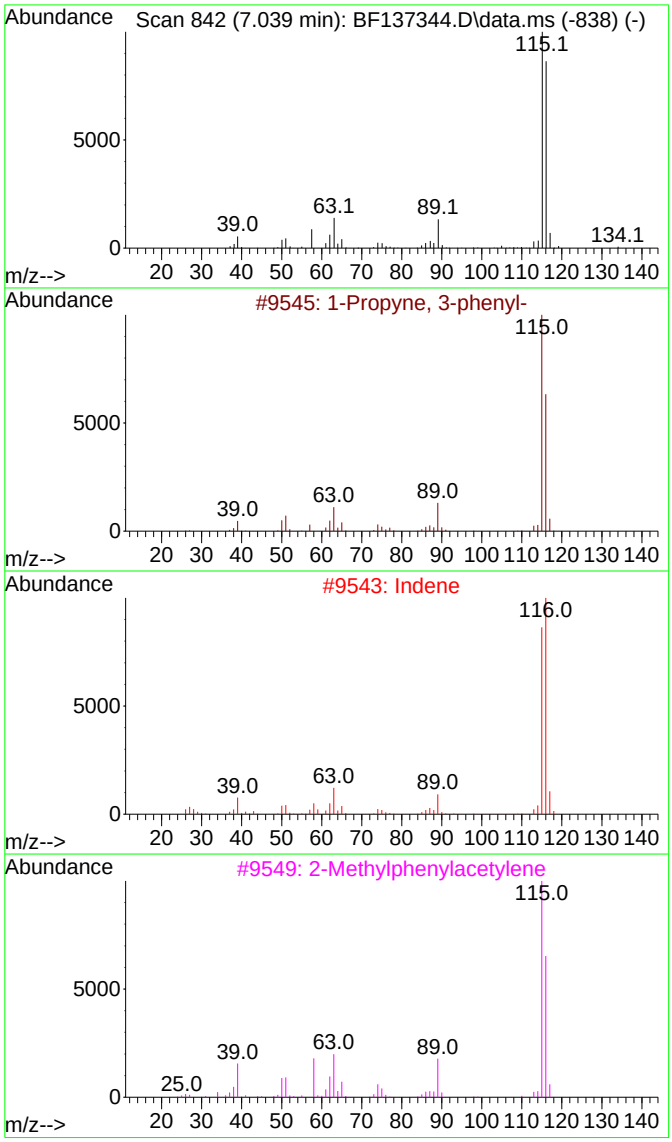
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

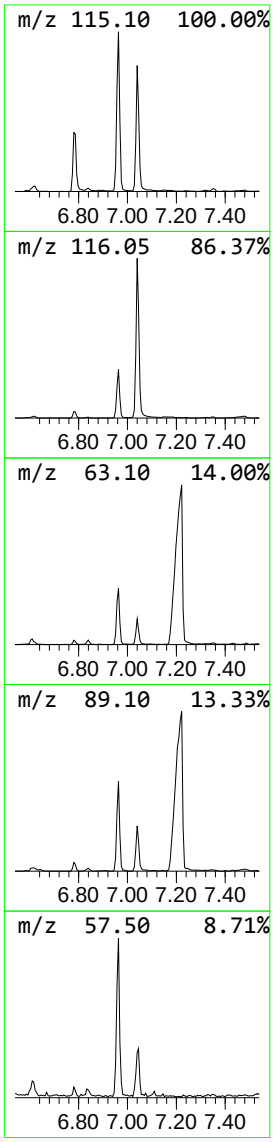
****

Peak Number 6 1-Propyne, 3-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.039	11.68 ng	347864	1,4-Dichlorobenzene-d4	6.787

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	94
3	2-Methylphenylacetylene	116	C9H8	000766-47-2	91
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 : 12 Sample Multiplier: 1

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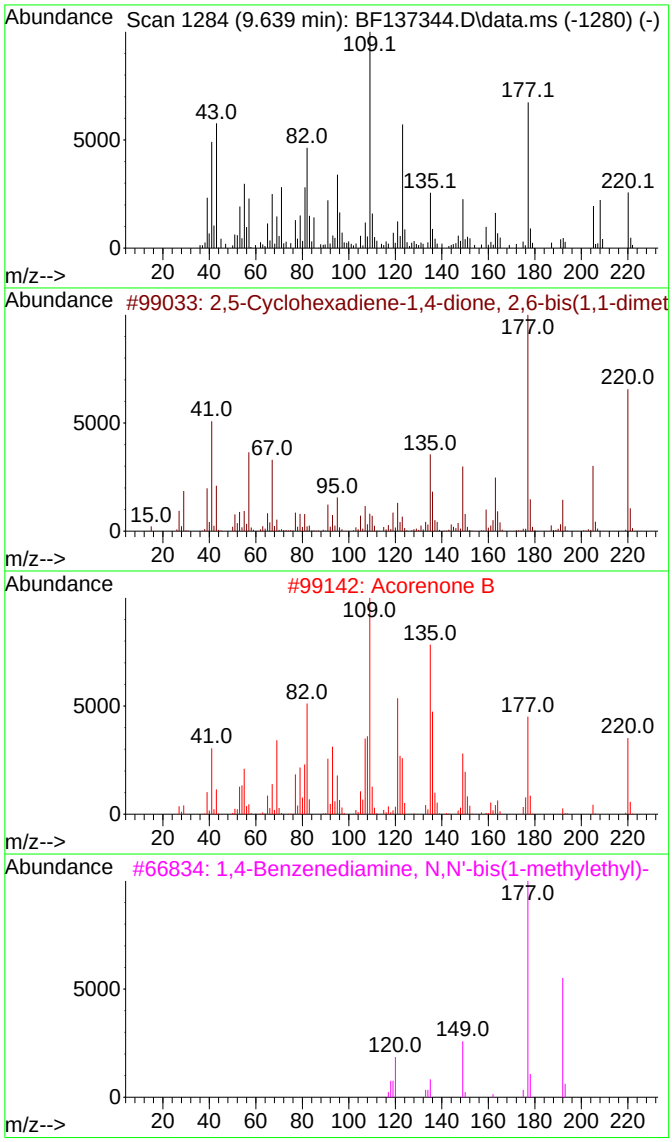
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

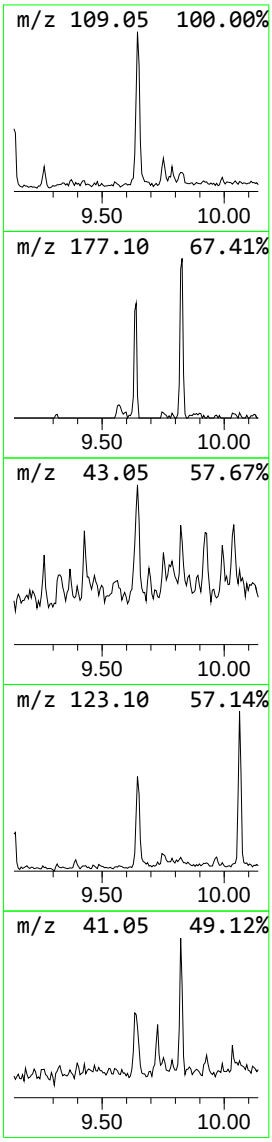
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.639	2.98 ng	186899	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	55
2	Acorenone B	220	C15H24O	021653-33-8	49
3	1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	25
4	2,5,5,6,8a-Pentamethyl-trans-4a,...	208	C14H24O	1000215-77-8	20
5	2-Propenamide, N-(4-methoxyphenyl)-	177	C10H11NO2	007766-37-2	15





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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
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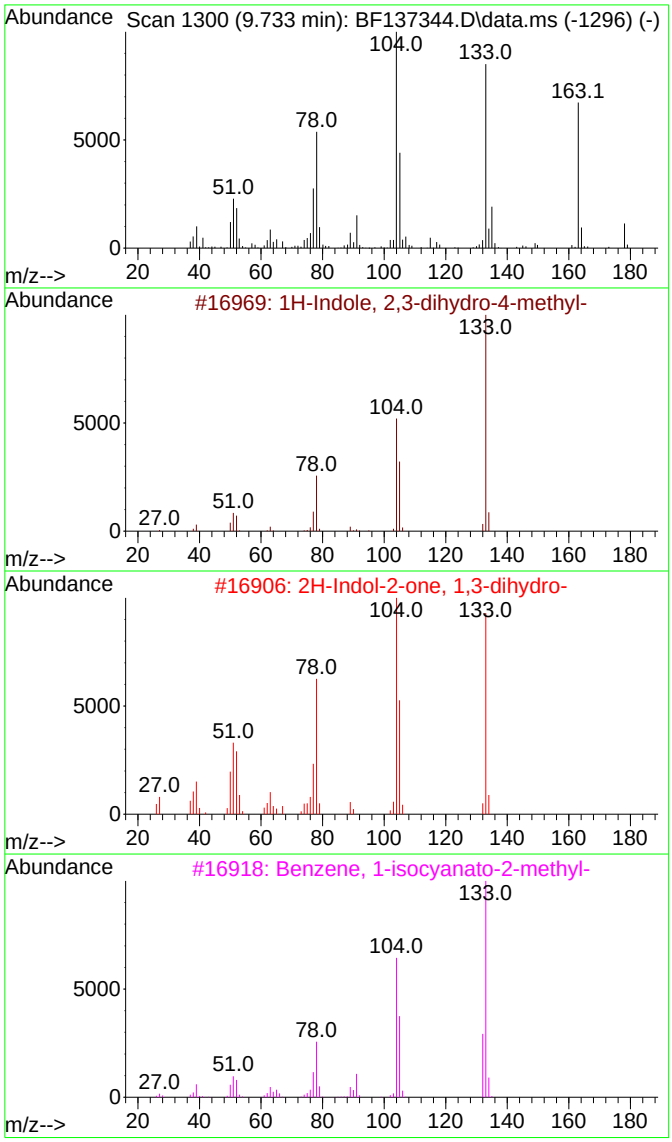
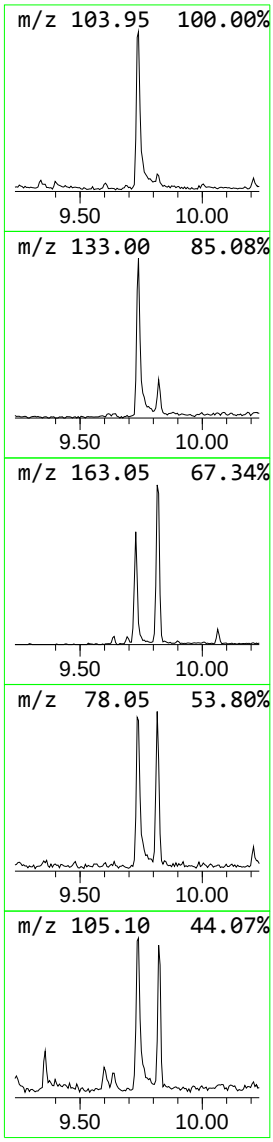
****
Peak Number 8 1H-Indole, 2,3-dihydro-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	4.21 ng	263643	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	062108-16-1	92
2	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	92
3	Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	89
4	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	70
5	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	70





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TIC Library : C:\Database\NIST20.L
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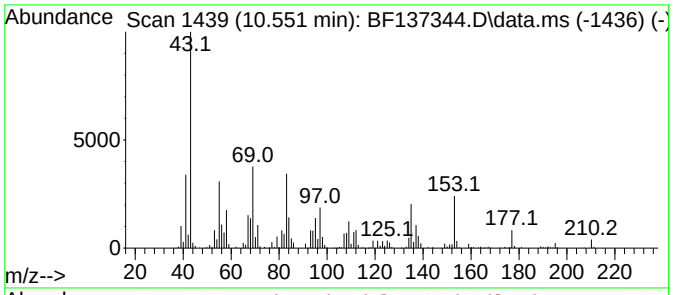
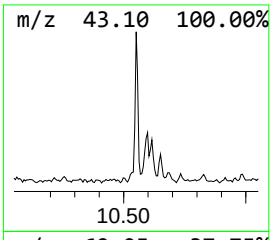
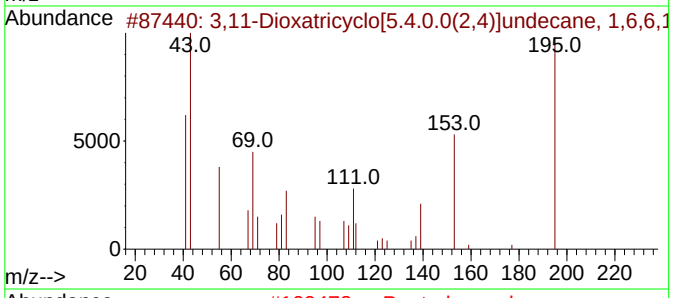
Peak Number 9 unknown10.551 Concentration Rank 11

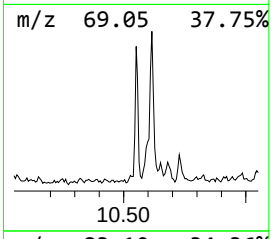
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	4.91 ng	307380	Acenaphthene-d10	9.816

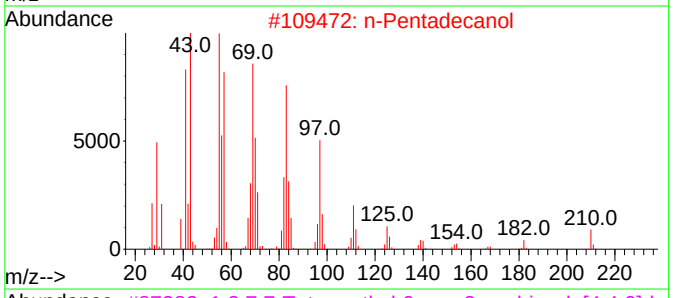
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,11-Dioxatricyclo[5.4.0.0(2,4)]...	210	C13H22O2	1000138-62-3	38
2	n-Pentadecanol	228	C15H32O	000629-76-5	22
3	1,3,7,7-Tetramethyl-9-oxo-2-oxab...	210	C13H22O2	005835-18-7	20
4	2,6,8-Trimethyl-4-nonyl acetate	228	C14H28O2	1000430-73-9	14
5	1-Pentadecene	210	C15H30	013360-61-7	10

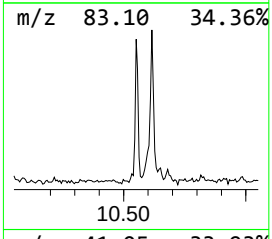


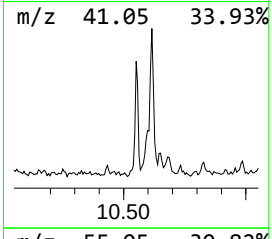


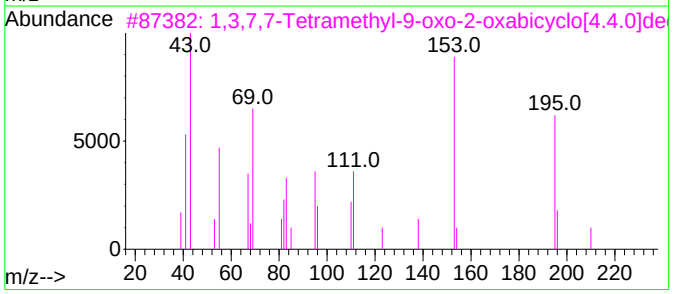


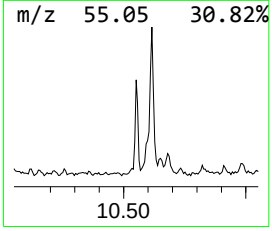












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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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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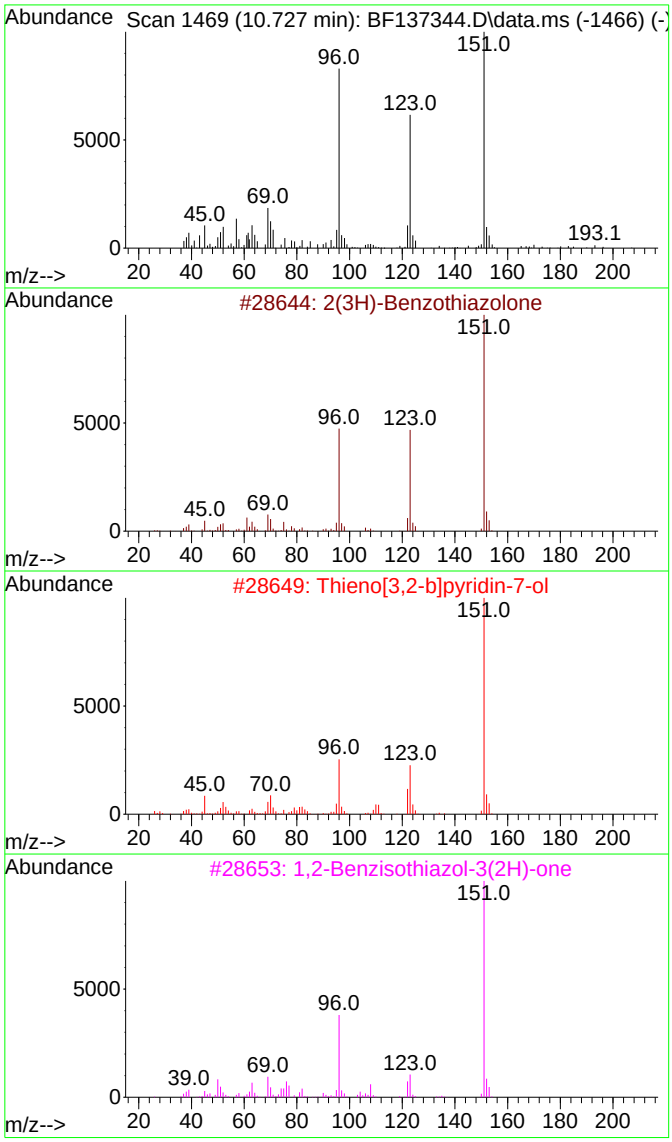
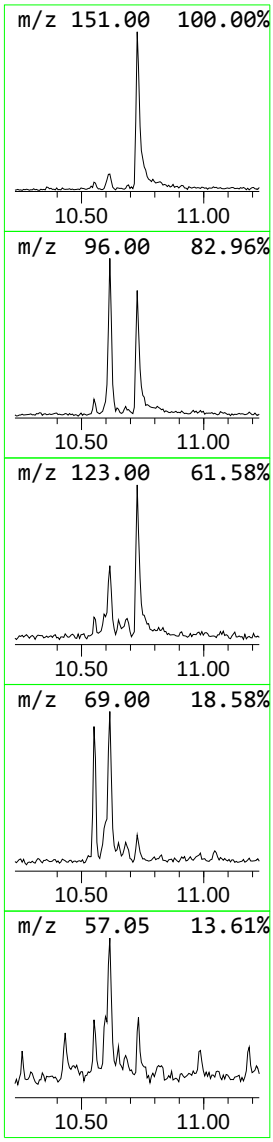
Peak Number 10 2(3H)-Benzothiazolone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.727	4.06 ng	160586	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	95
2	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	49
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	46
4	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	43
5	t-Butylhydroquinone	166	C10H14O2	001948-33-0	43





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Data File : BF137344.D
Acq On : 08 Feb 2024 18:19
Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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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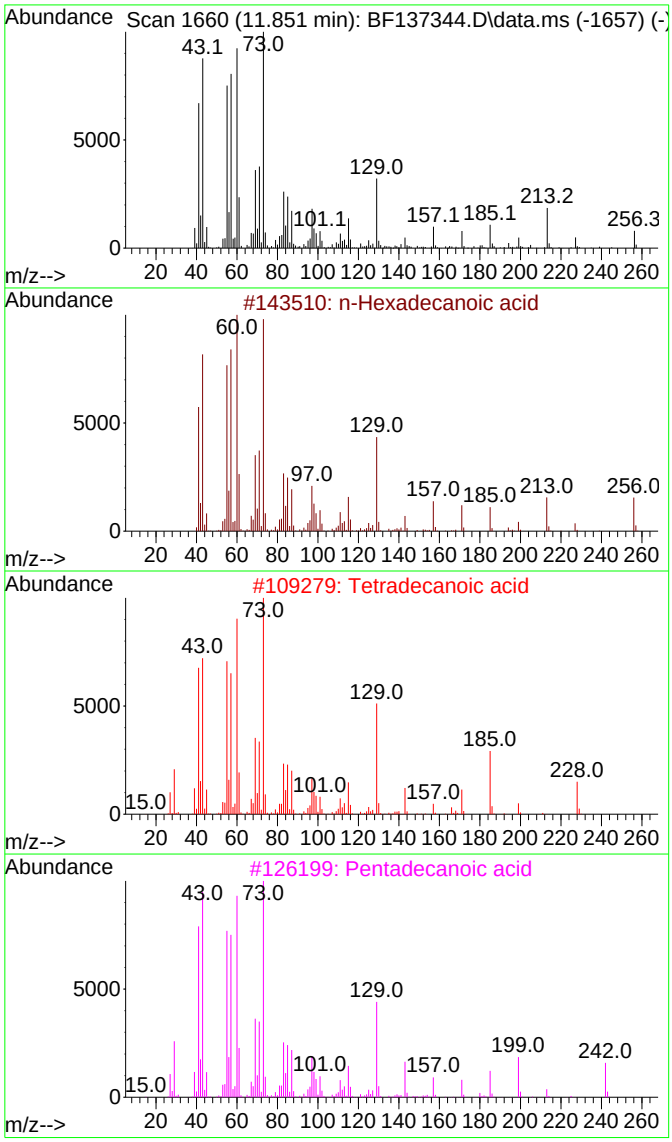
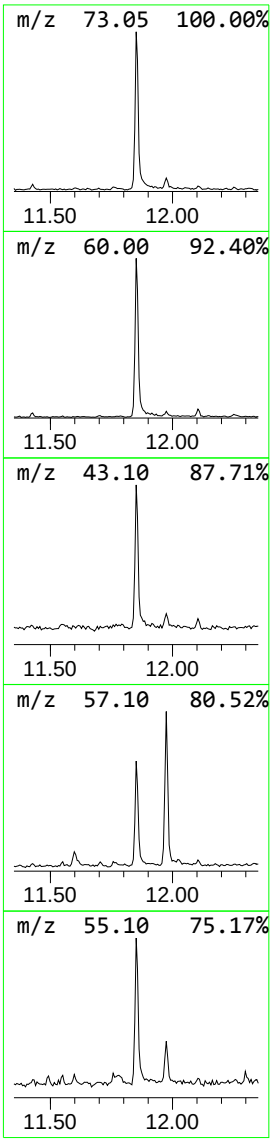
Peak Number 11 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	11.85 ng	469127	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	Octanoic acid	144	C8H16O2	000124-07-2	60





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Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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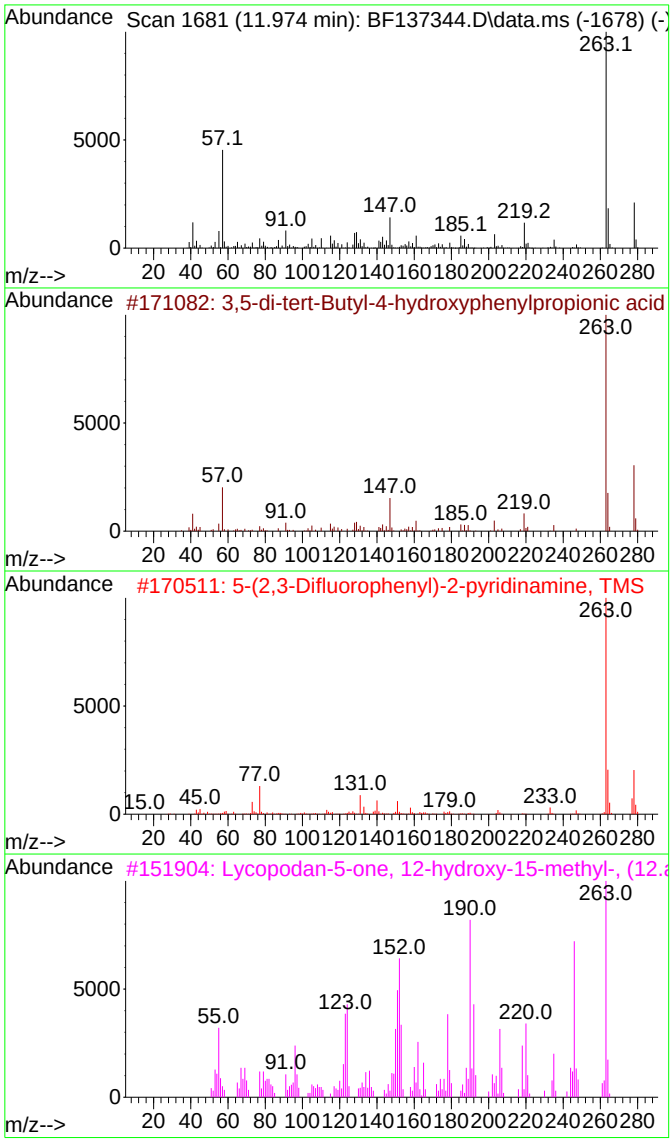
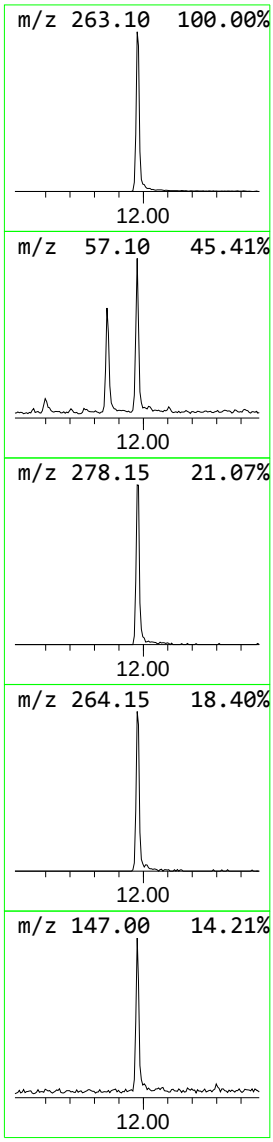
Peak Number 12 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	12.40 ng	490731	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	96
2	5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	81
3	Lycopodan-5-one, 12-hydroxy-15-m...	263	C16H25NO2	021061-90-5	60
4	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	59
5	2,6-Bis(tert-butyl)phenol, TMS d...	278	C17H30OSi	010416-73-6	59





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Data File : BF137344.D
Acq On : 08 Feb 2024 18:19
Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
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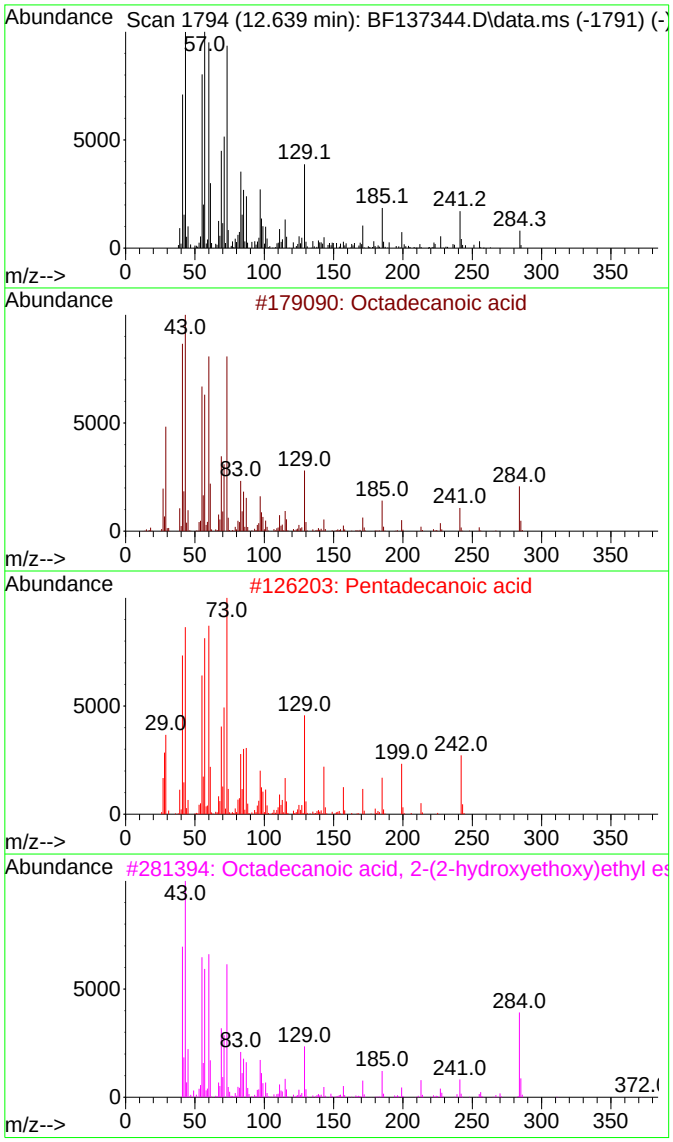
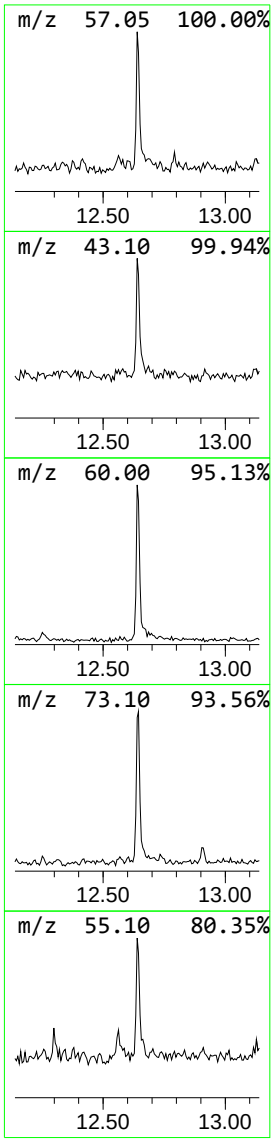
Peak Number 13 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	5.98 ng	160921	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Pentadecane	212	C15H32	000629-62-9	25





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Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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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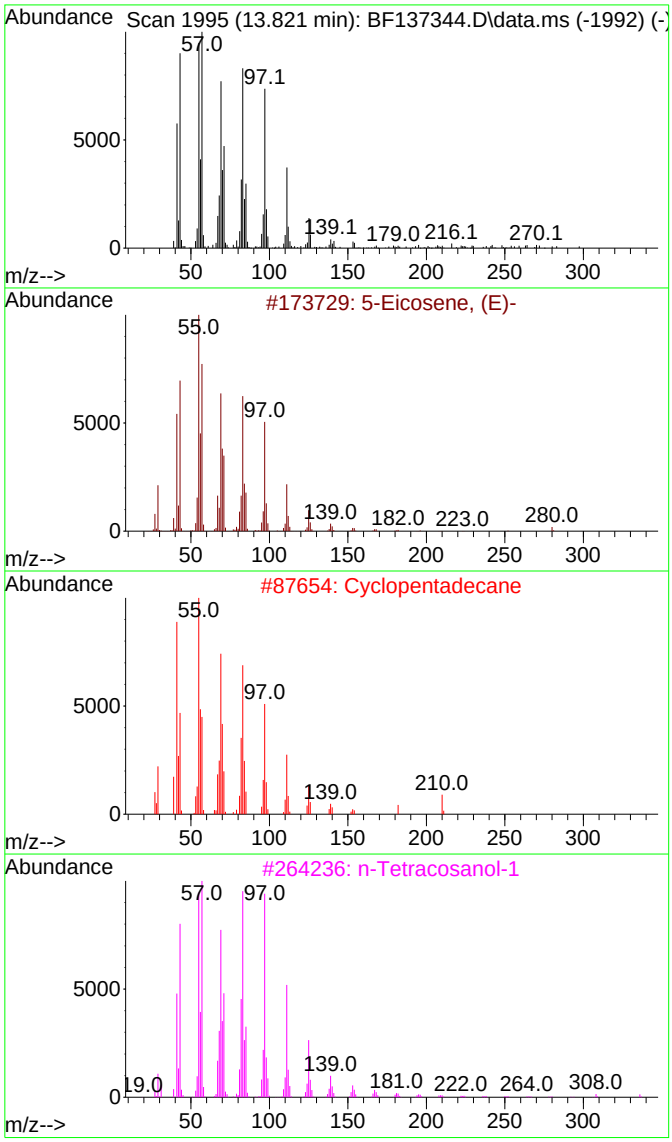
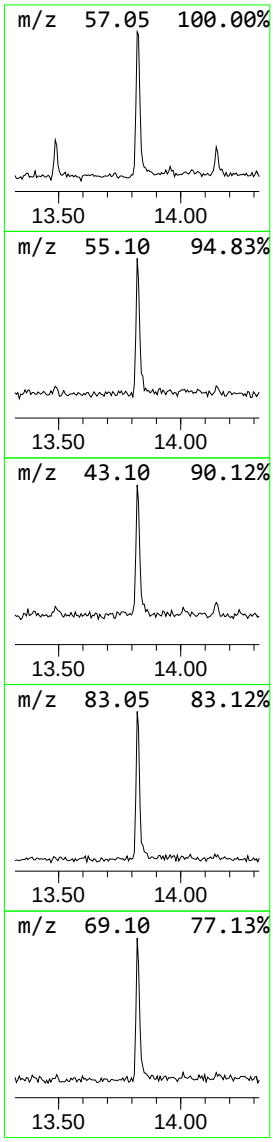
Peak Number 14 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	9.46 ng	254754	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Cyclopentadecane	210	C15H30	000295-48-7	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137344.D
Acq On : 08 Feb 2024 18:19
Operator : CG\JU
Sample : P1372-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CG-MW-17-ch7

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, 1,3-di...	5.640	16.7	ng	497126	1	6.787	595672	20.0
Benzene, 1,2,3-...	6.839	5.8	ng	173080	1	6.787	595672	20.0
Indane	6.963	41.6	ng	1240190	1	6.787	595672	20.0
1-Propyne, 3-ph...	7.039	11.7	ng	347864	1	6.787	595672	20.0
2,5-Cyclohexadi...	9.639	3.0	ng	186899	3	9.816	1252930	20.0
1H-Indole, 2,3-...	9.733	4.2	ng	263643	3	9.816	1252930	20.0
unknown10.551	10.551	4.9	ng	307380	3	9.816	1252930	20.0
2(3H)-Benzothia...	10.727	4.1	ng	160586	4	11.310	791544	20.0
n-Hexadecanoic ...	11.851	11.9	ng	469127	4	11.310	791544	20.0
3,5-di-tert-But...	11.974	12.4	ng	490731	4	11.310	791544	20.0
Octadecanoic acid	12.639	6.0	ng	160921	5	13.963	538533	20.0
5-Eicosene, (E)-	13.821	9.5	ng	254754	5	13.963	538533	20.0