

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
 Data File : BG054294.D
 Acq On : 15 Jul 2022 00:40
 Operator : CG/JU
 Sample : N3688-03 10X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-240

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_G\Methods\8270-BG071222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.041	785	792	801	rVB	78317	135898	8.00%	1.432%
2	10.850	1258	1270	1279	rBV	104678	224868	13.23%	2.369%
3	11.901	1441	1449	1452	rBV7	18682	44463	2.62%	0.468%
4	11.948	1453	1457	1464	rVB6	25468	51936	3.06%	0.547%
5	12.301	1511	1517	1520	rBV7	22006	52051	3.06%	0.548%
6	12.583	1560	1565	1570	rBV4	35590	70774	4.16%	0.746%
7	12.647	1572	1576	1583	rVV8	14479	43857	2.58%	0.462%
8	12.753	1590	1594	1599	rBV	44481	80245	4.72%	0.845%
9	12.830	1604	1607	1612	rBV5	25072	49015	2.88%	0.516%
10	13.123	1652	1657	1662	rVB3	69235	116565	6.86%	1.228%
11	13.464	1710	1715	1723	rBV3	161123	291503	17.15%	3.071%
12	13.946	1794	1797	1801	rBV5	79999	121418	7.15%	1.279%
13	14.016	1803	1809	1813	rVV3	131895	322716	18.99%	3.400%
14	14.105	1819	1824	1829	rBV	536129	883404	51.99%	9.308%
15	14.422	1873	1878	1884	rBV7	280878	700780	41.24%	7.383%
16	14.516	1889	1894	1900	rVB	720339	1280502	75.35%	13.491%
17	14.651	1911	1917	1929	rBV9	501164	1699329	100.00%	17.904%
18	15.197	2007	2010	2014	rBV3	259326	405351	23.85%	4.271%
19	15.479	2053	2058	2064	rVB2	798047	1363682	80.25%	14.368%
20	21.701	3113	3117	3122	rVB2	272148	425601	25.05%	4.484%
21	22.553	3258	3262	3269	rVB	319170	559482	32.92%	5.895%
22	24.933	3659	3667	3683	rVB2	179563	567809	33.41%	5.982%

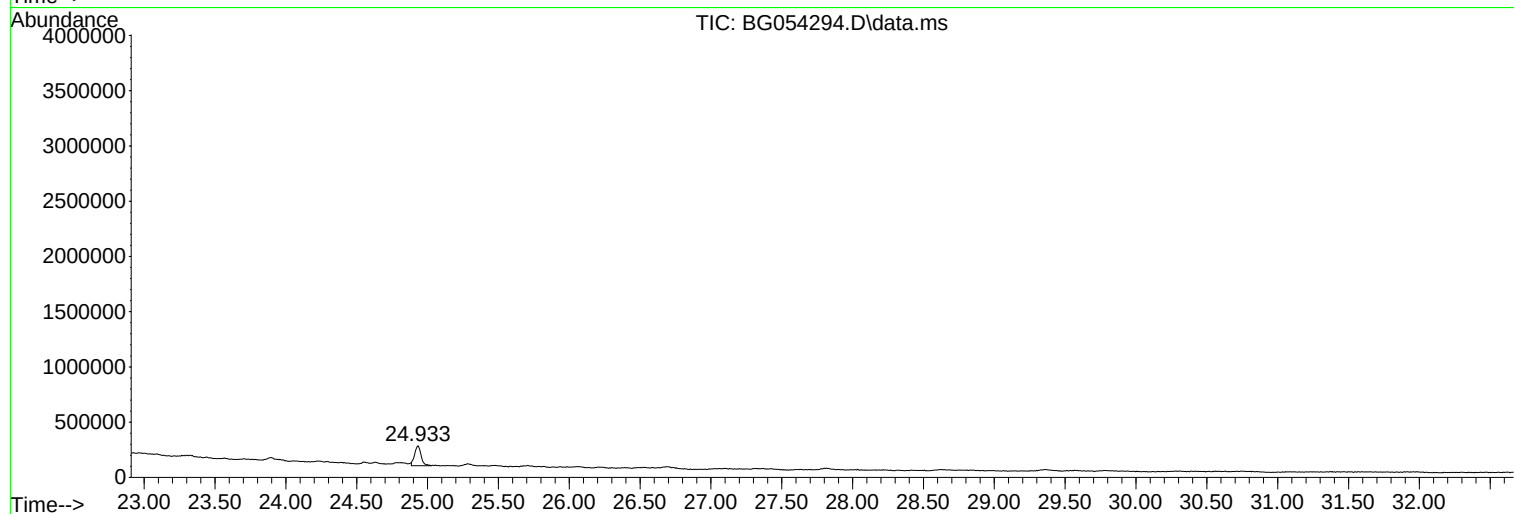
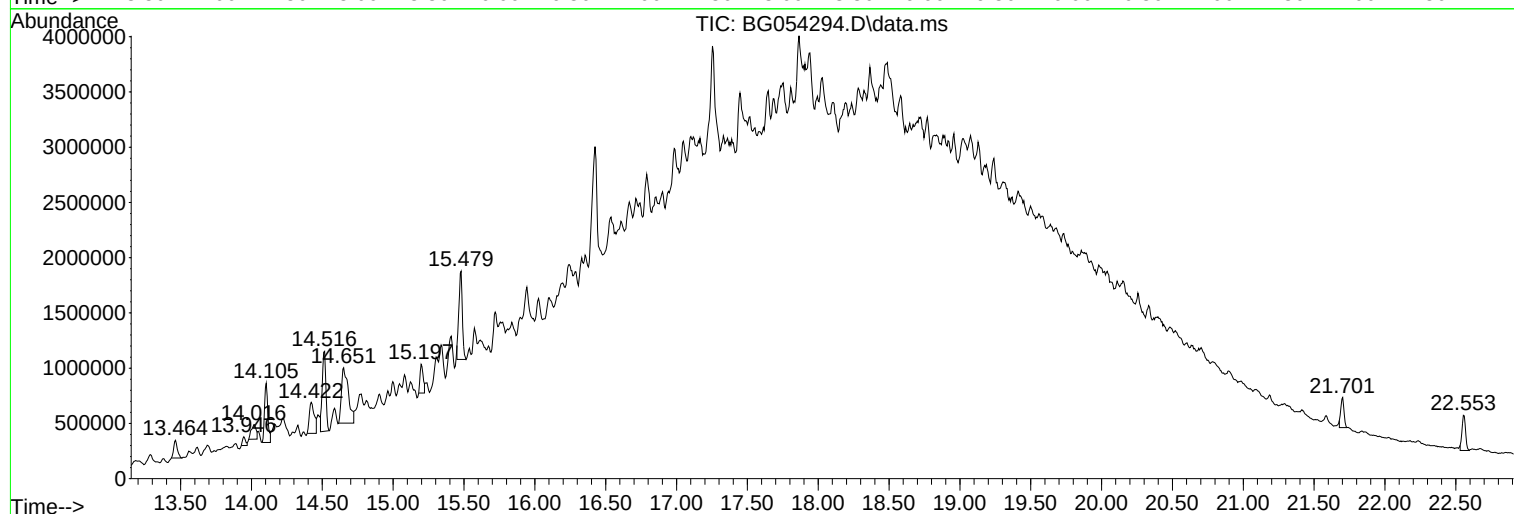
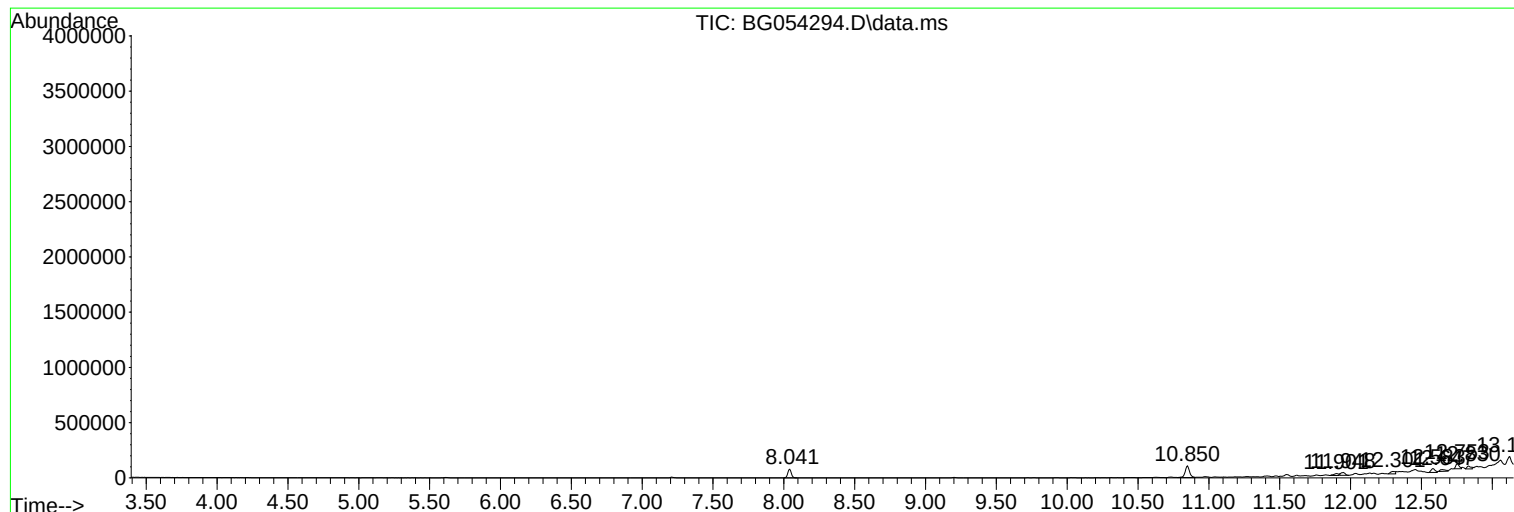
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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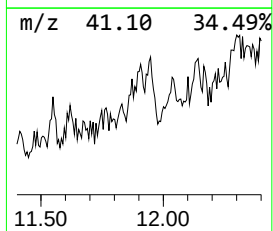
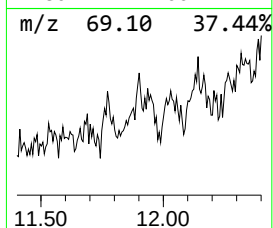
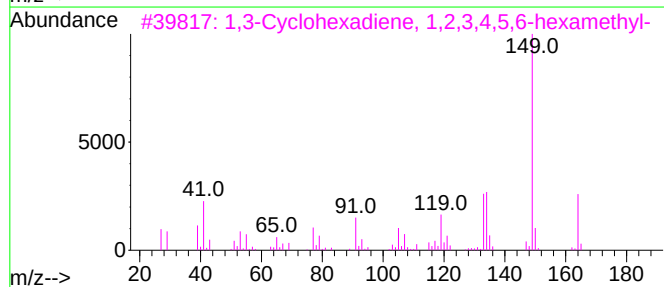
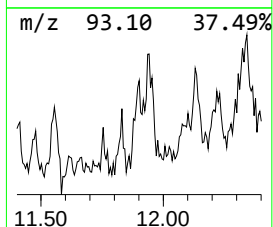
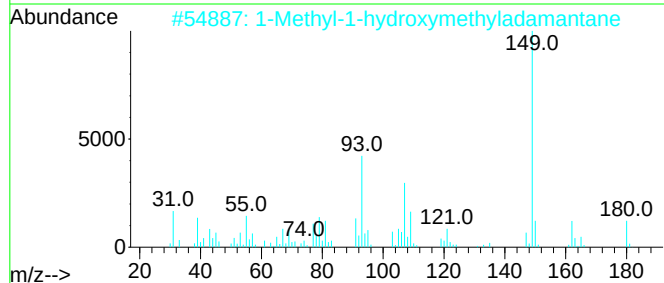
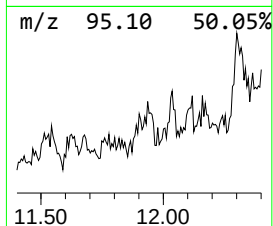
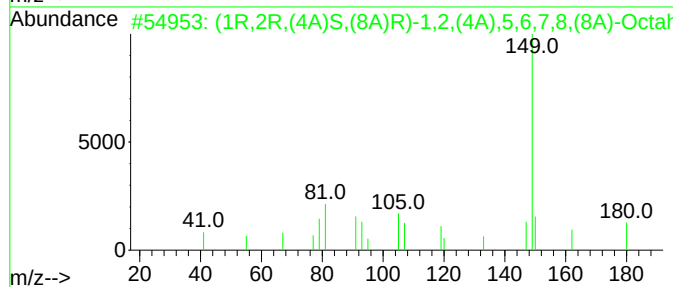
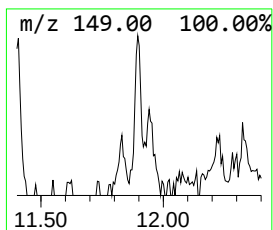
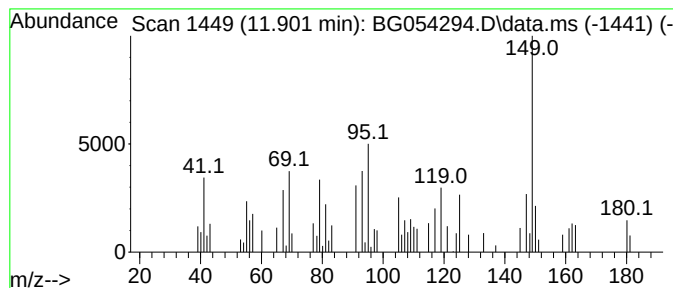
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (1R,2R,(4A)S,(8A)R)-1,2,(4A... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.901	3.95 ng	44463	Naphthalene-d8	10.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1R,2R,(4A)S,(8A)R)-1,2,(4A),5,6...	180	C12H20O	1000434-46-5	55
2			1-Methyl-1-hydroxymethyladamantane	180	C12H20O	001200-78-8	45
3			1,3-Cyclohexadiene, 1,2,3,4,5,6-...	164	C12H20	1000152-09-6	35
4			2-t-Butyl-6-[2-hydroxy-2-(2,4,6-...	318	C19H26O4	1010192-88-0	32
5			Phthalic acid, 3-bromobenzyl eth...	362	C17H15BrO4	1000371-05-6	27



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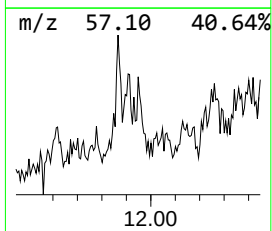
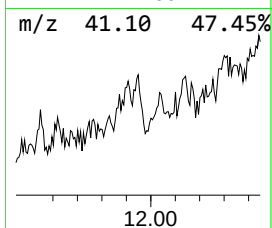
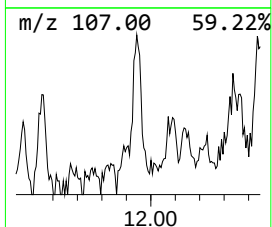
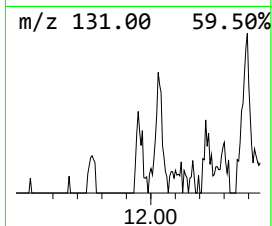
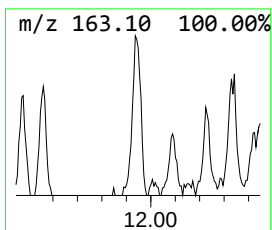
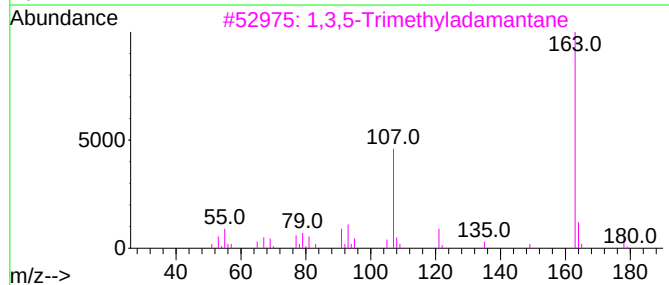
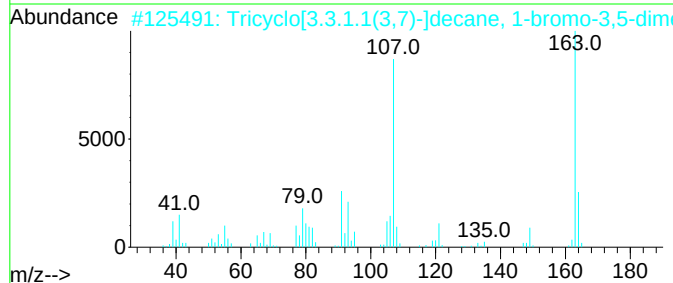
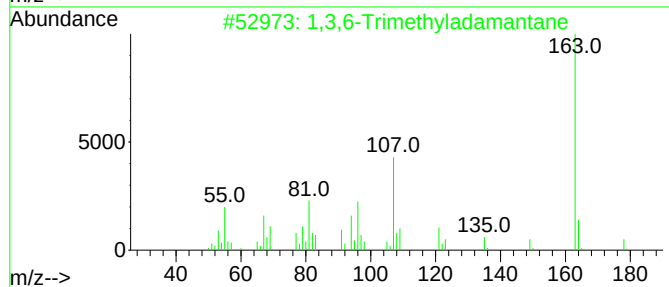
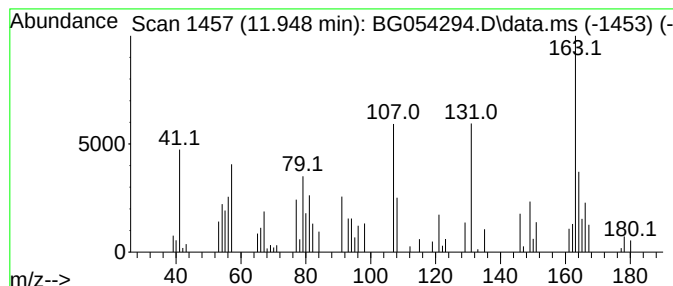
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown11.948 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.948	4.62 ng	51936	Naphthalene-d8	10.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	43
2			Tricyclo[3.3.1.1(3,7)-]decane, 1...	242	C12H19Br	000941-37-7	43
3			1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	38
4			1,3,3-Trimethyl-2-(2-methyl-cycl...	178	C13H22	285129-06-8	32
5			benzoxazole, 7-methoxy-2-methyl-	163	C9H9NO2	1000404-43-8	32



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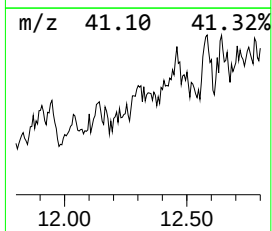
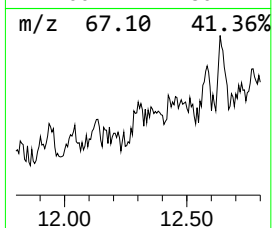
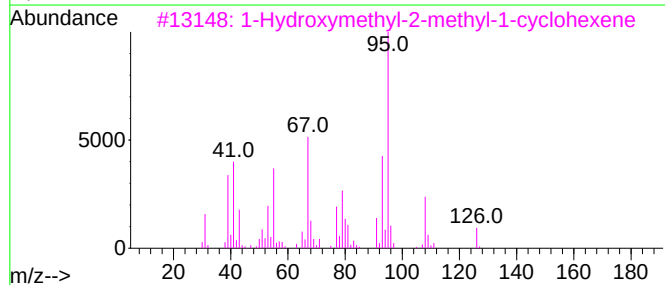
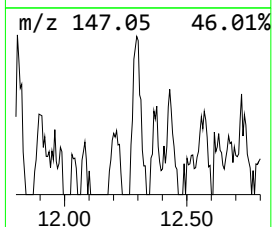
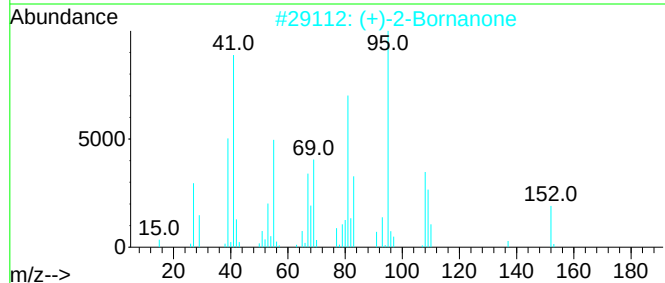
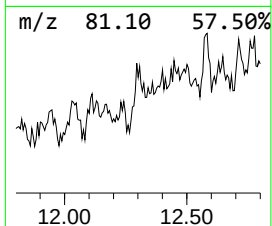
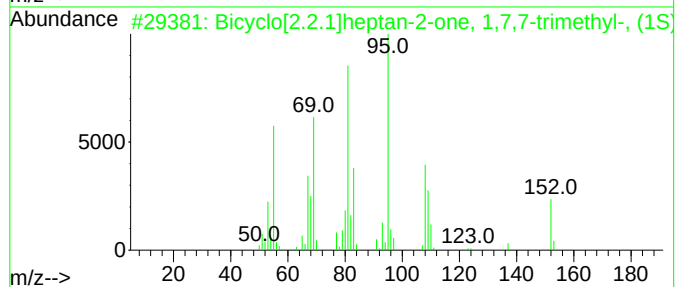
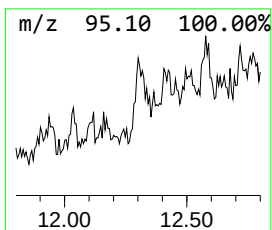
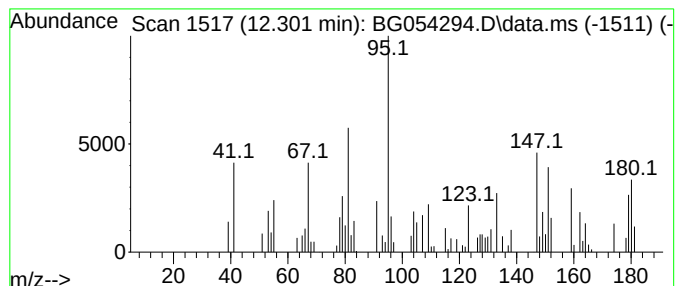
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.301 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	4.63 ng	52051	Naphthalene-d8	10.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	38
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	30
3			1-Hydroxymethyl-2-methyl-1-cyclo...	126	C8H14O	029474-11-1	30
4			5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	27
5			Ethanone, 1-bicyclo[2.2.1]hept-2...	138	C9H14O	000824-59-9	27



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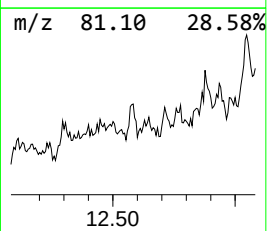
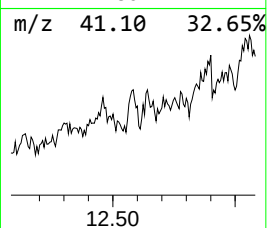
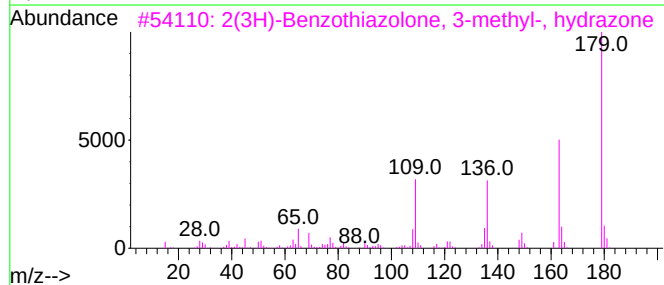
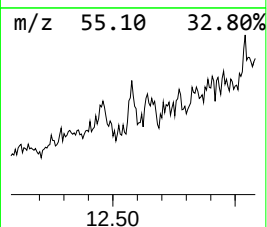
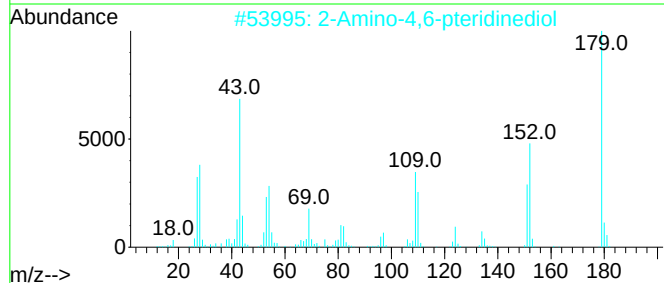
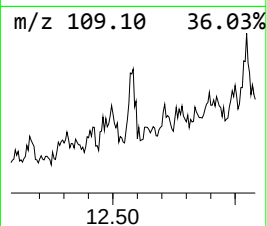
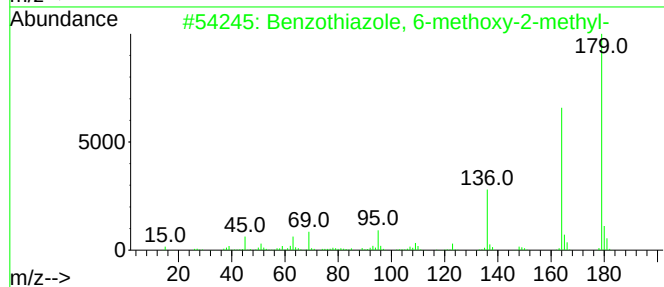
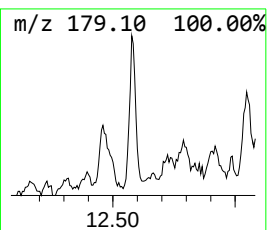
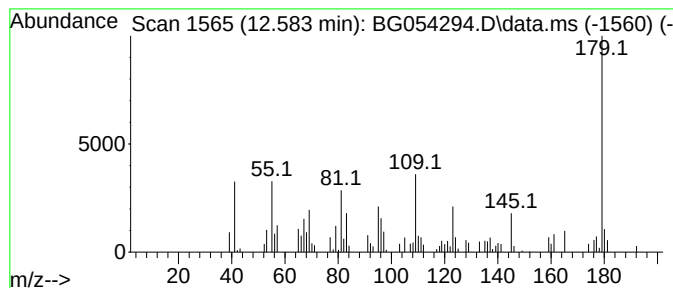
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.583 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.583	6.29 ng	70774	Naphthalene-d8	10.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzothiazole, 6-methoxy-2-methyl-	179	C9H9NOS	002941-72-2	43
2			2-Amino-4,6-pteridinediol	179	C6H5N5O2	005979-01-1	43
3			2(3H)-Benzothiazolone, 3-methyl-...	179	C8H9N3S	001128-67-2	43
4			2,4-Dimethoxyphenyl isocyanate	179	C9H9NO3	084370-87-6	38
5			Imidazolo[1,2-a]pyrimidine-2,5(1...	179	C8H9N3O2	053854-19-6	38



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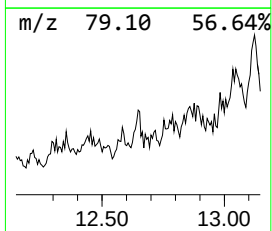
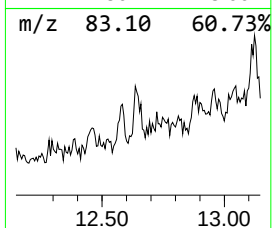
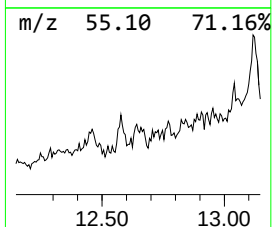
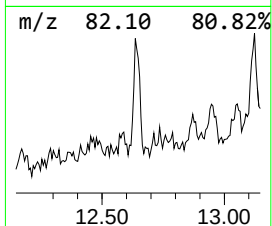
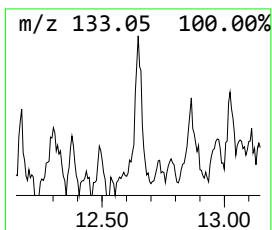
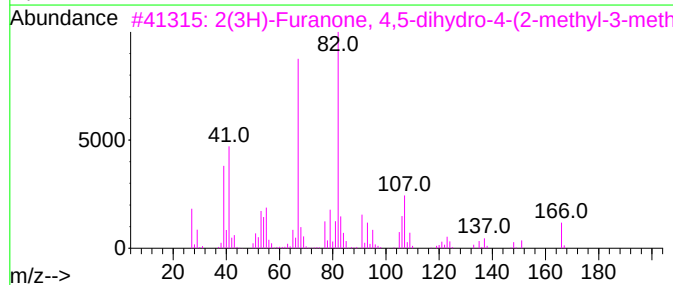
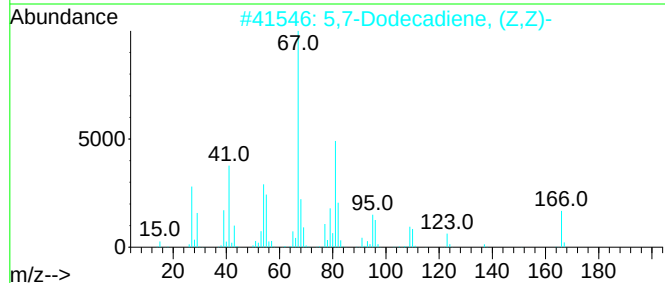
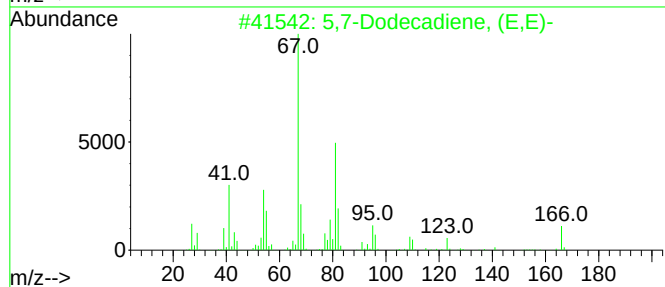
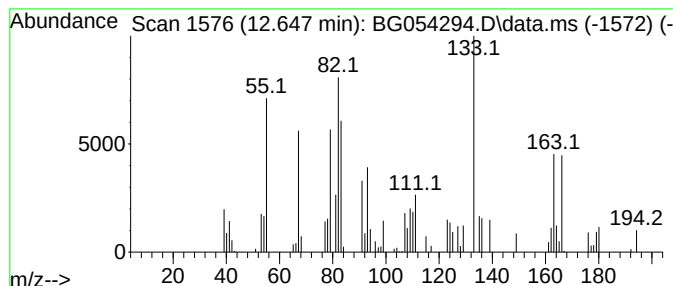
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown12.647 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.647	3.90 ng	43857	Naphthalene-d8	10.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,7-Dodecadiene, (E,E)-	166	C12H22	030651-68-4	27
2			5,7-Dodecadiene, (Z,Z)-	166	C12H22	006108-62-9	22
3			2(3H)-Furanone, 4,5-dihydro-4-(2-methyl-3-methyl-2-butyl)-	166	C10H14O2	1000153-91-5	22
4			1,1'-Bicyclohexyl	166	C12H22	000092-51-3	22
5			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	22



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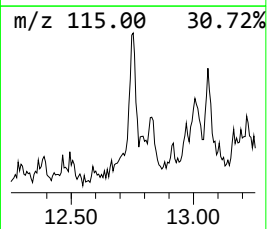
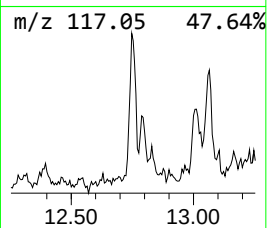
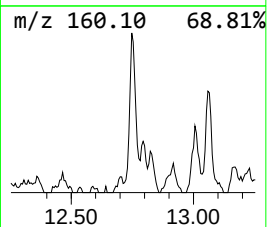
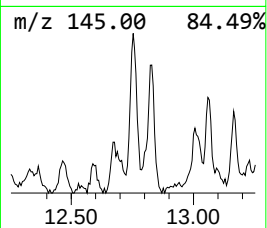
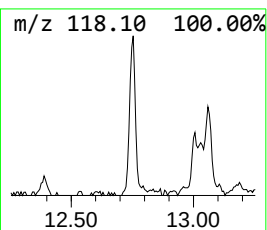
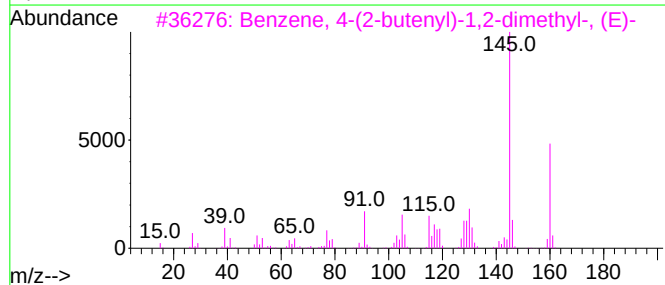
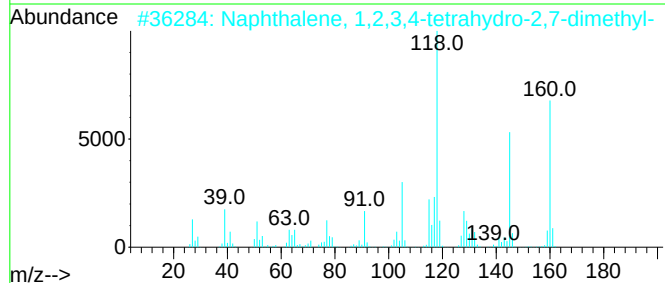
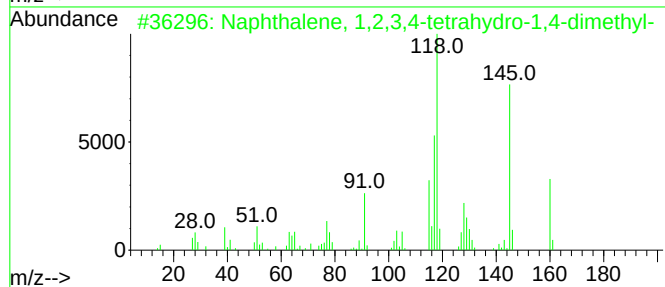
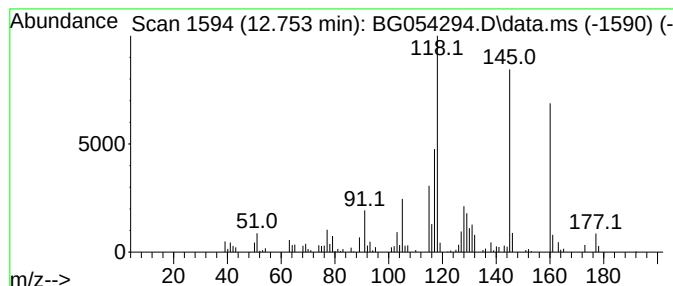
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.753	7.14 ng	80245	Naphthalene-d8	10.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	81
3			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	78
4			4-Chloro-3-fluoroanisole	160	C7H6ClFO	000501-29-1	60
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
Operator : CG/JU
Sample : N3688-03 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-240

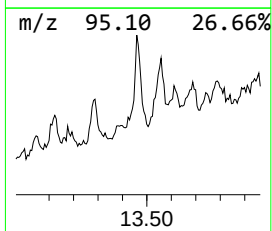
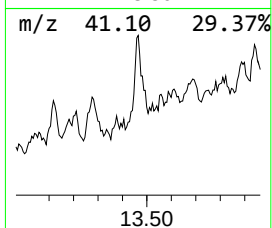
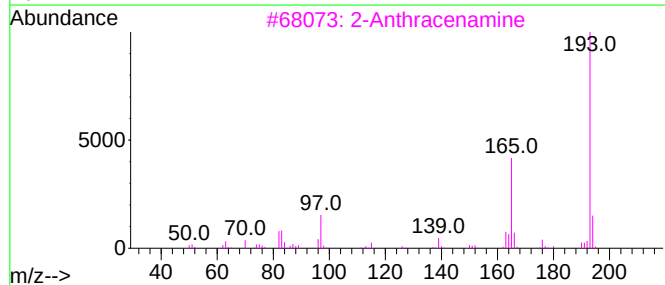
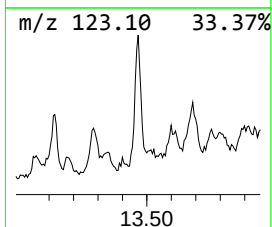
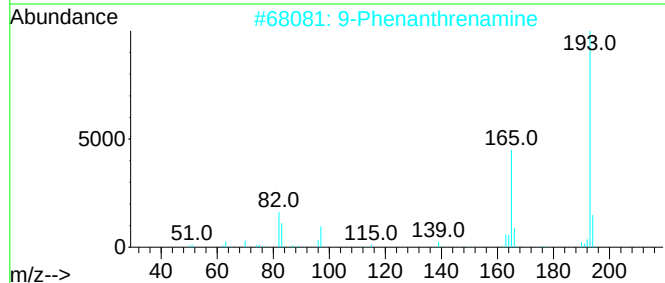
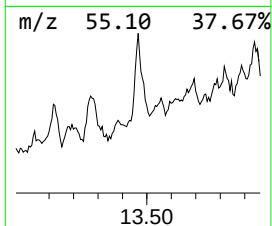
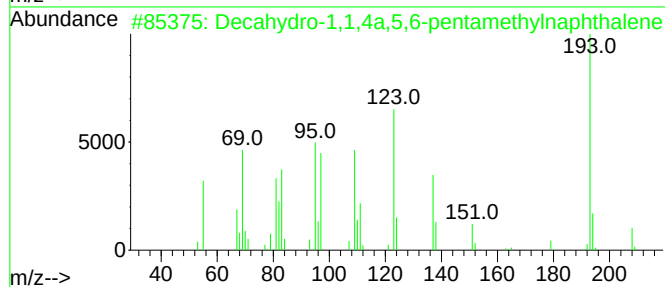
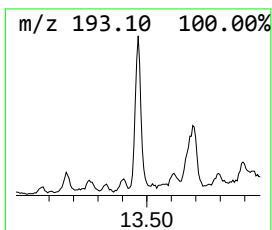
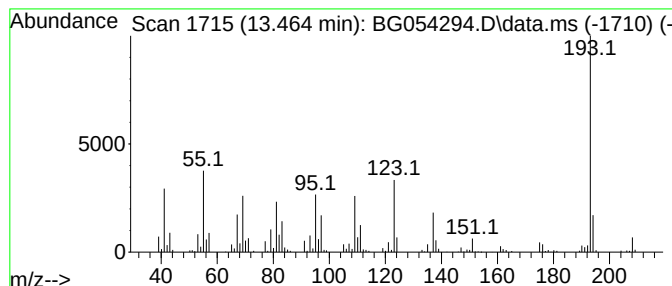
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	3.43 ng	291503	Acenaphthene-d10	14.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	92
2			9-Phenanthrenamine	193	C14H11N	000947-73-9	46
3			2-Anthracenamine	193	C14H11N	000613-13-8	43
4			2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	43
5			Pyrazole, 5-methyl-3-(5-nitro-2...	193	C8H7N3O3	016239-90-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
Operator : CG/JU
Sample : N3688-03 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-240

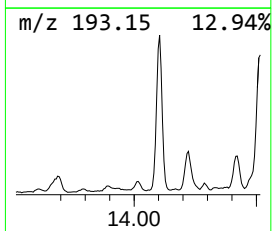
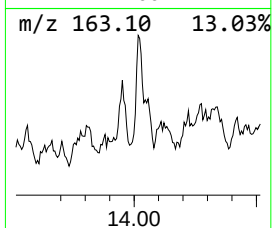
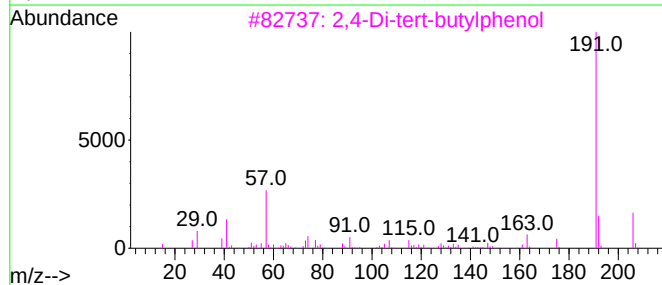
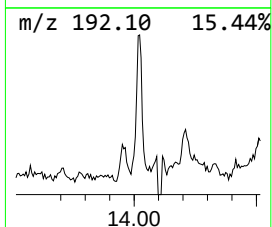
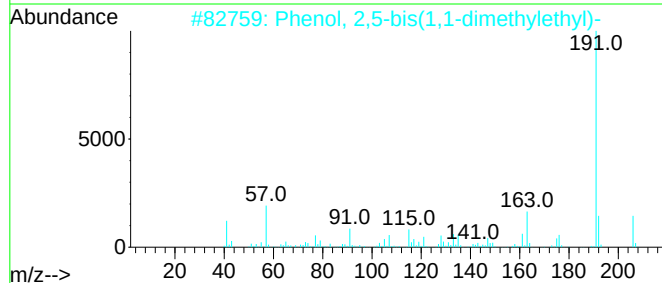
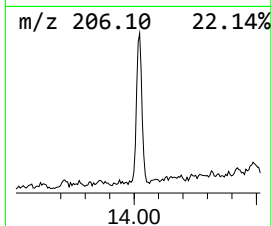
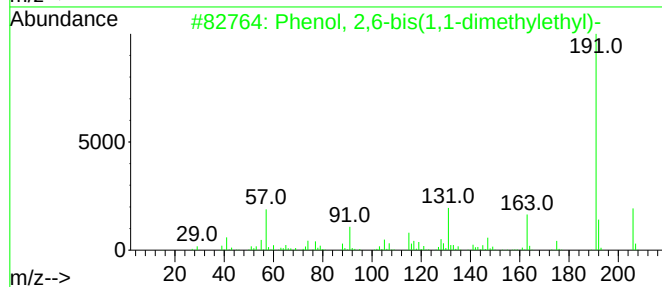
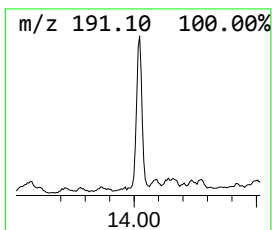
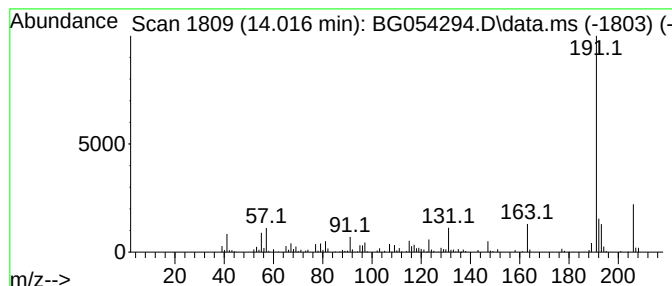
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	3.80 ng	322716	Acenaphthene-d10	14.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	87
2			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	64
3			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	64
4			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	59
5			4H-Benzo[def]carbazole	191	C14H9N	000203-65-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
Operator : CG/JU
Sample : N3688-03 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

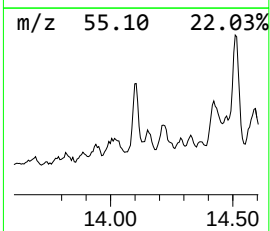
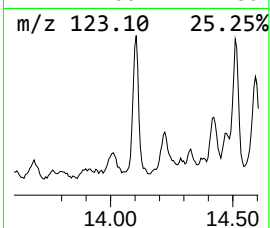
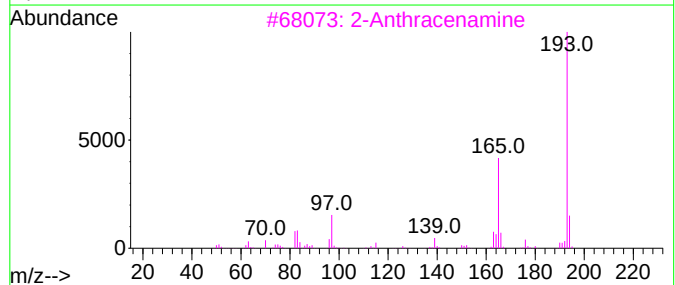
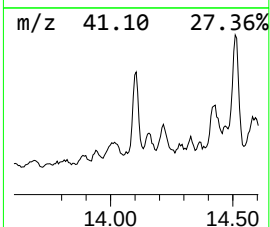
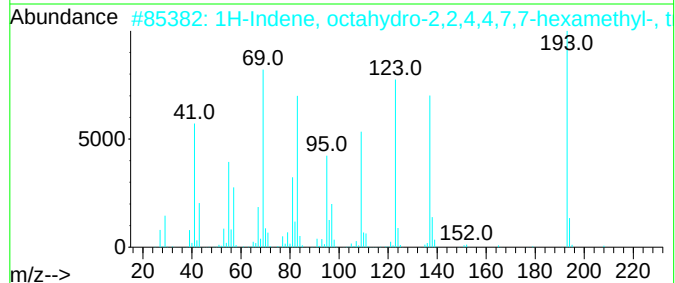
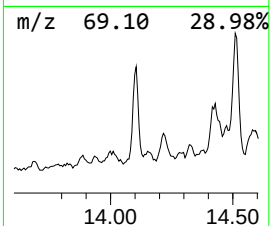
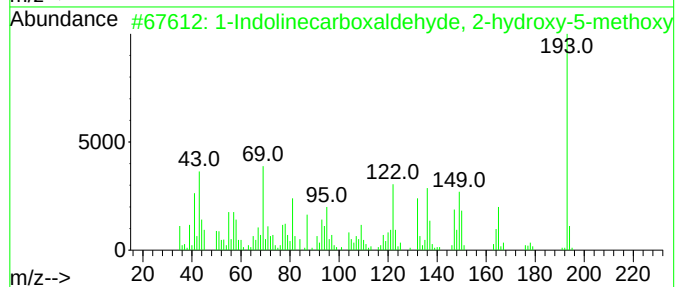
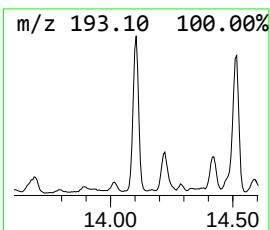
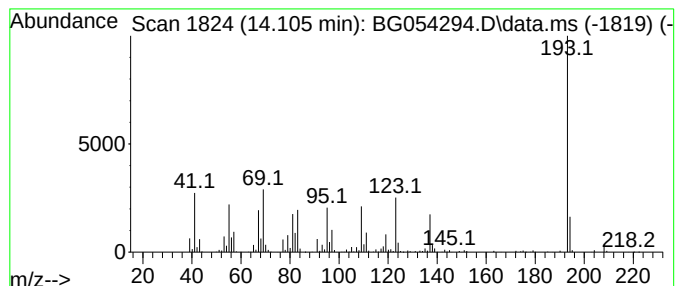
Instrument :
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ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Indolinecarboxaldehyde, 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.105	10.40 ng	883404	Acenaphthene-d10		14.674	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Indolinecarboxaldehyde, 2-hydr...		193	C10H11NO3	013303-70-3	50
2	1H-Indene, octahydro-2,2,4,4,7,7...		208	C15H28	054832-83-6	38
3	2-Anthracenamine		193	C14H11N	000613-13-8	38
4	1-Anthracenamine		193	C14H11N	000610-49-1	38
5	Trisiloxane, 1,1,3,3,5,5-hexamet...		208	C6H20O2Si3	001189-93-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
Operator : CG/JU
Sample : N3688-03 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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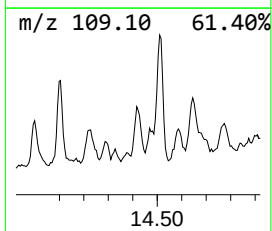
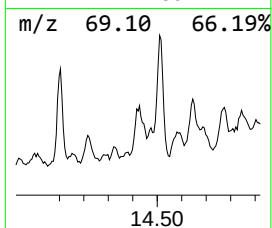
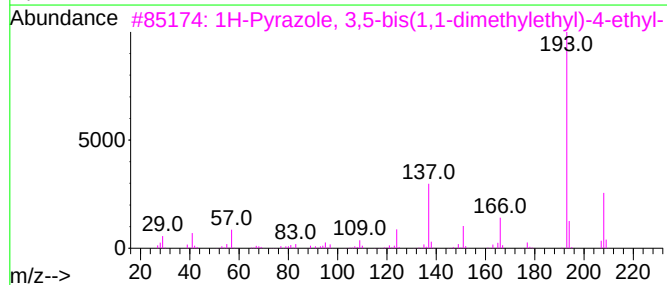
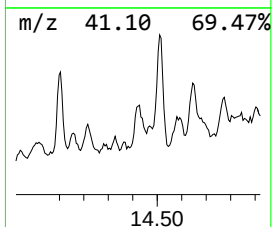
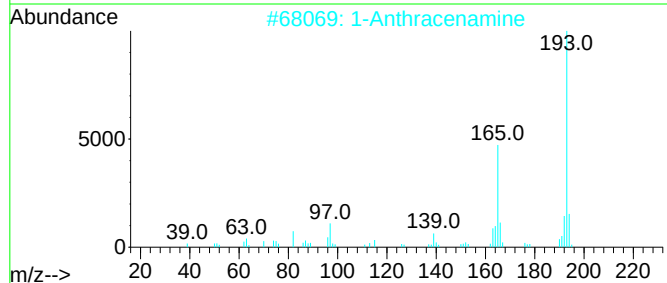
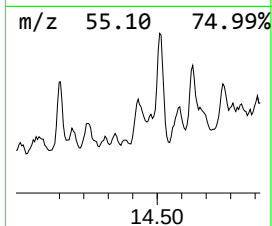
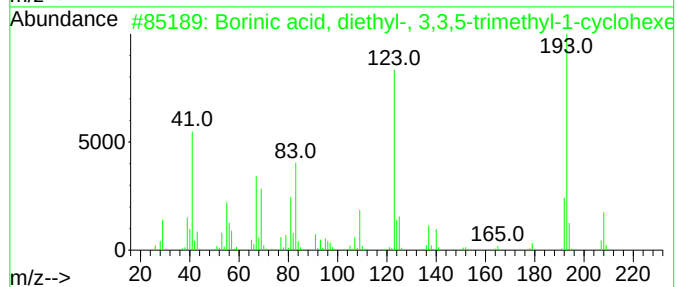
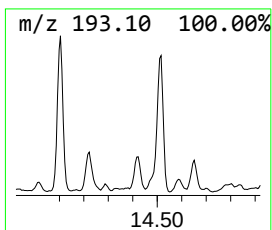
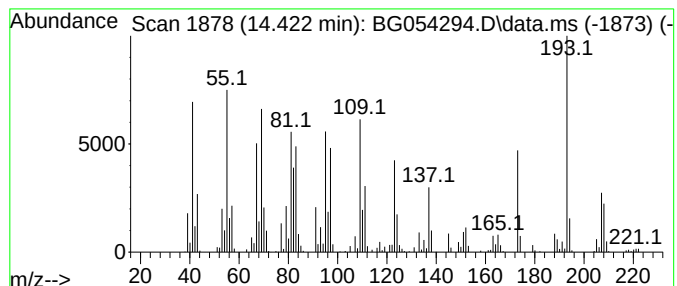
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.422 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	8.25 ng	700780	Acenaphthene-d10	14.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
2			1-Anthracenamine	193	C14H11N	000610-49-1	38
3			1H-Pyrazole, 3,5-bis(1,1-dimethy...	208	C13H24N2	125281-21-2	30
4			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
5			Iminostilbene	193	C14H11N	000256-96-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
Operator : CG/JU
Sample : N3688-03 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

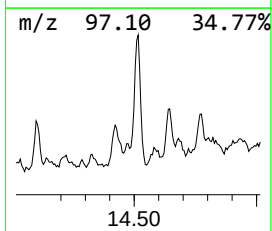
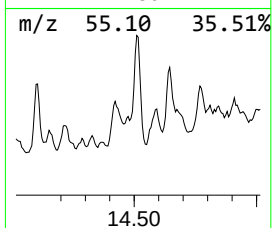
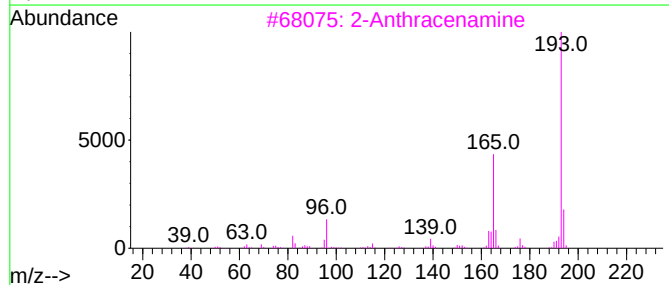
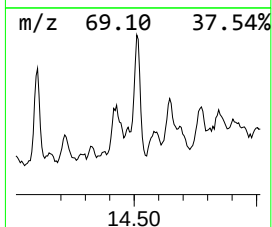
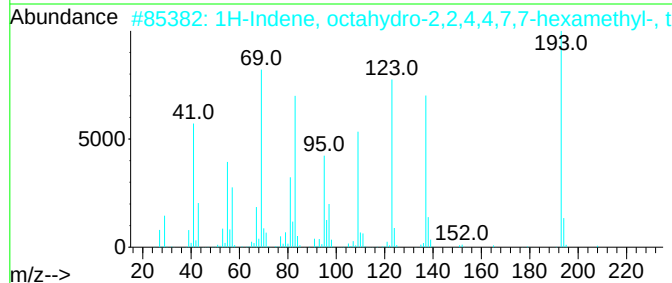
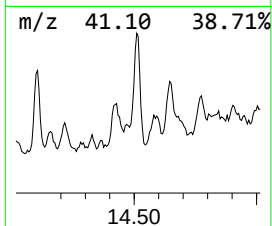
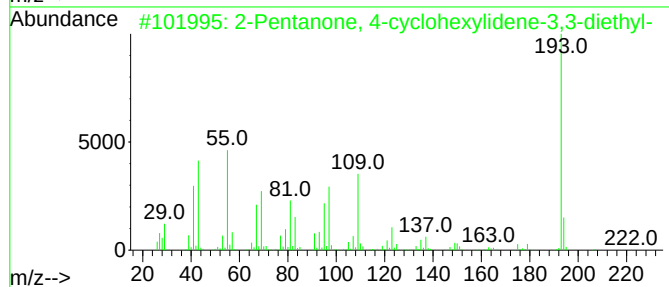
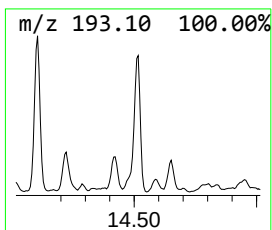
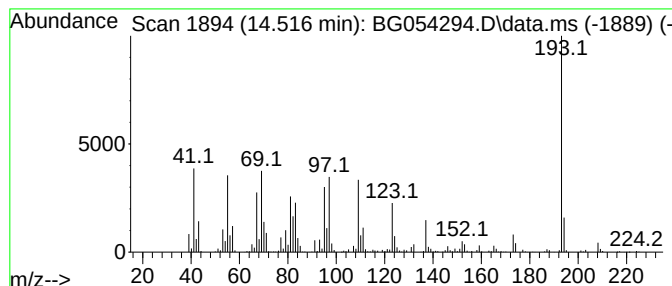
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ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Pentanone, 4-cyclohexylid... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.516	15.07 ng	1280500	Acenaphthene-d10	14.674
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		2-Pentanone, 4-cyclohexylidene-3...	222 C15H26O	313253-65-5 64
2		1H-Indene, octahydro-2,2,4,4,7,7...	208 C15H28	054832-83-6 40
3		2-Anthracenamine	193 C14H11N	000613-13-8 38
4		Decahydro-1,1,4a,5,6-pentamethyl...	208 C15H28	080655-44-3 38
5		9-Phenanthrenamine	193 C14H11N	000947-73-9 38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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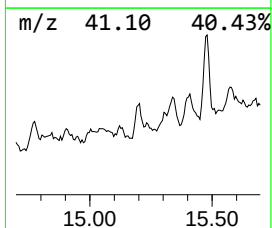
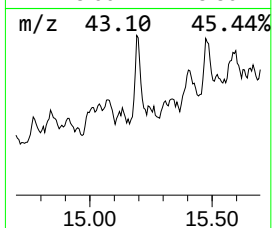
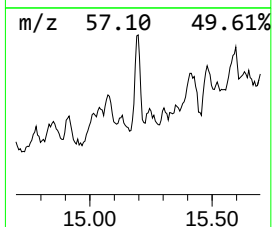
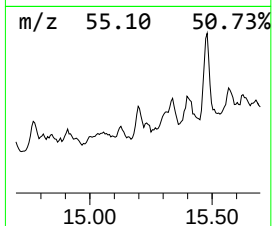
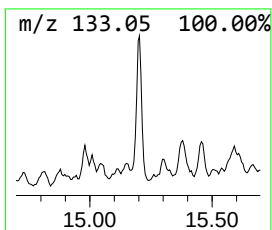
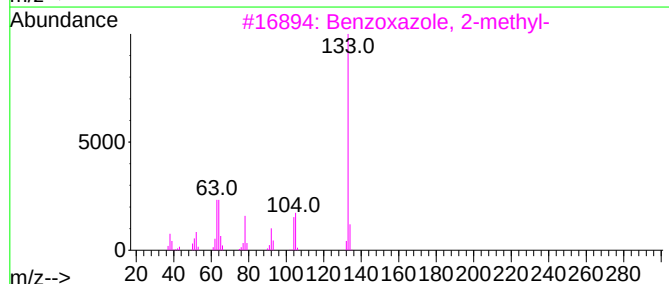
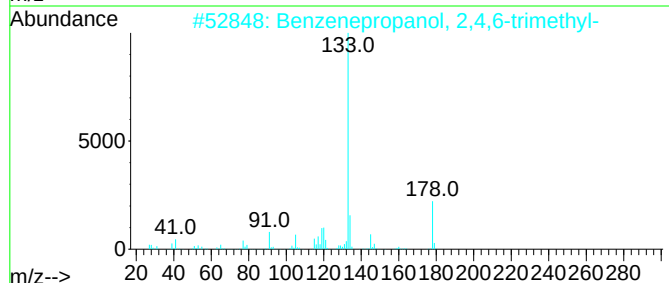
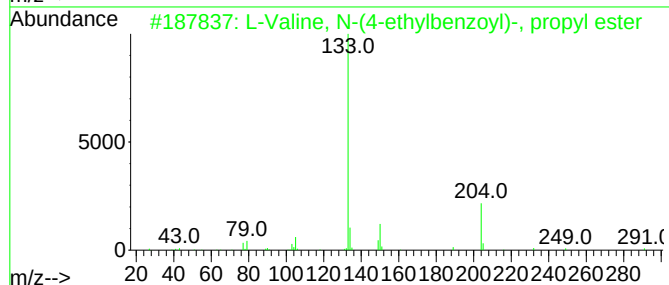
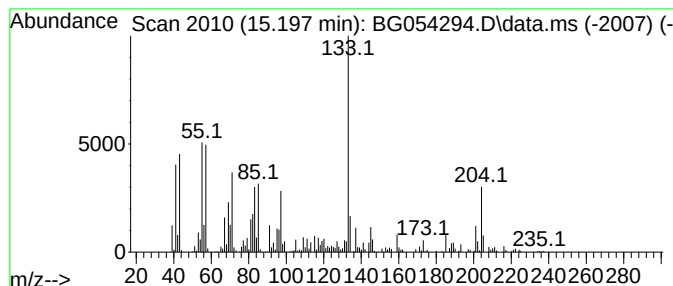
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.197 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.197	4.77 ng	405351	Acenaphthene-d10	14.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Valine, N-(4-ethylbenzoyl)-, p...	291	C17H25NO3	1000346-62-9	43
2			Benzenepropanol, 2,4,6-trimethyl-	178	C12H18O	027645-07-4	38
3			Benzoxazole, 2-methyl-	133	C8H7NO	000095-21-6	35
4			4-Ethylbenzoic acid, 2-methyloct...	272	C18H24O2	1010292-54-5	35
5			6-Aminoindazole	133	C7H7N3	006967-12-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
Data File : BG054294.D
Acq On : 15 Jul 2022 00:40
Operator : CG/JU
Sample : N3688-03 10X
Misc :
ALS Vial : 16 Sample Multiplier: 1

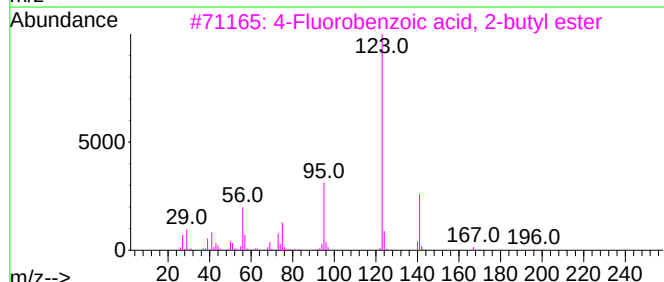
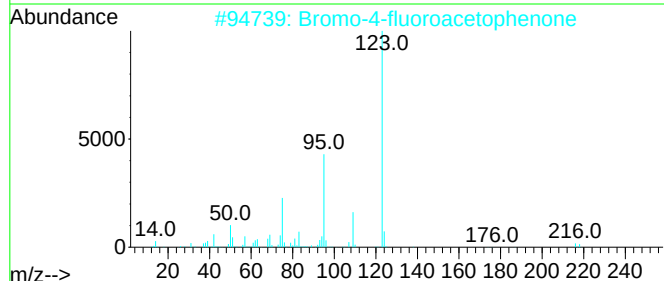
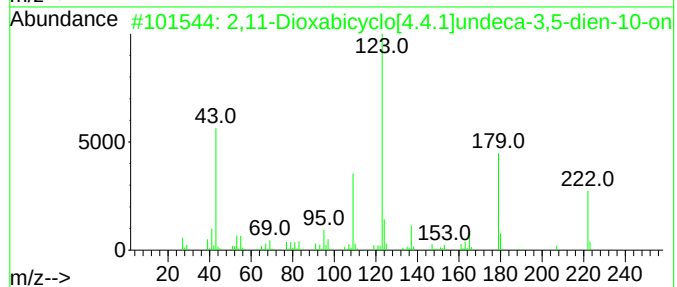
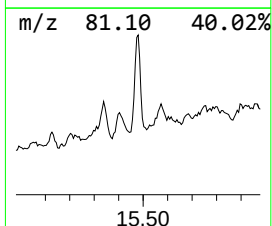
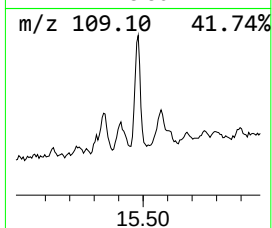
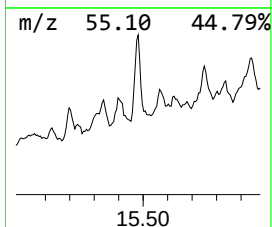
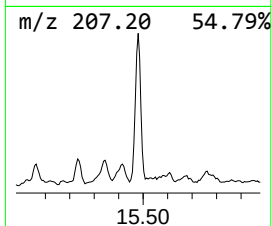
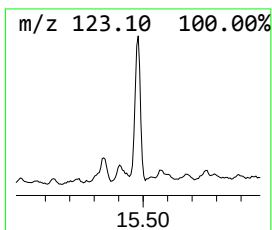
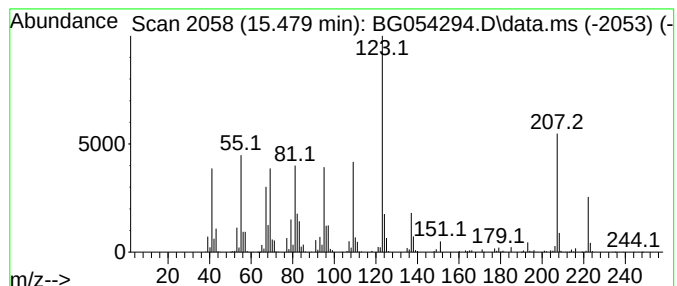
Instrument :
BNA_G
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.479	16.05 ng	1363680	Acenaphthene-d10			14.674
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...		222	C13H18O3	070412-52-1	50
2	Bromo-4-fluoroacetophenone		216	C8H6BrFO	000403-29-2	38
3	4-Fluorobenzoic acid, 2-butyl ester		196	C11H13FO2	090172-12-6	38
4	2-Fluorobenzoic acid, 2-ethylcyc...		250	C15H19FO2	1000278-98-1	38
5	Pyridine-3-carboxylic acid, 1-[(...		290	C15H18N2O4	1010310-27-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071422\
 Data File : BG054294.D
 Acq On : 15 Jul 2022 00:40
 Operator : CG/JU
 Sample : N3688-03 10X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071222.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(1R,2R,(4A)S,(8...	11.901	4.0	ng	44463	2	10.850	224868	20.0
unknown11.948	11.948	4.6	ng	51936	2	10.850	224868	20.0
unknown12.301	12.301	4.6	ng	52051	2	10.850	224868	20.0
unknown12.583	12.583	6.3	ng	70774	2	10.850	224868	20.0
unknown12.647	12.647	3.9	ng	43857	2	10.850	224868	20.0
Naphthalene, 1,...	12.753	7.1	ng	80245	2	10.850	224868	20.0
Decahydro-1,1,4...	13.464	3.4	ng	291503	3	14.674	1699330	20.0
Phenol, 2,6-bis...	14.016	3.8	ng	322716	3	14.674	1699330	20.0
1-Indolinecarbo...	14.105	10.4	ng	883404	3	14.674	1699330	20.0
unknown14.422	14.422	8.3	ng	700780	3	14.674	1699330	20.0
2-Pentanone, 4-...	14.516	15.1	ng	1280500	3	14.674	1699330	20.0
unknown15.197	15.197	4.8	ng	405351	3	14.674	1699330	20.0
2,11-Dioxabicyc...	15.479	16.1	ng	1363680	3	14.674	1699330	20.0
3-Acetyl-1-(3,4...	22.553	26.3	ng	559482	5	21.701	425601	20.0