

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
 Data File : BG053326.D
 Acq On : 26 Apr 2022 18:52
 Operator : CG/JU
 Sample : N2482-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COP-2R

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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.277	145	151	158	rVB	18425	32041	1.19%	0.351%
2	5.193	301	307	315	rBV2	25876	42238	1.57%	0.463%
3	5.410	339	344	353	rBV2	16175	27756	1.03%	0.304%
4	5.669	382	388	395	rBV	211233	345979	12.89%	3.795%
5	5.733	395	399	409	rVB2	16842	38255	1.43%	0.420%
6	6.109	458	463	469	rBV2	16815	28016	1.04%	0.307%
7	7.267	653	660	670	rBV	150340	282210	10.52%	3.095%
8	7.631	716	722	727	rBV2	17401	31236	1.16%	0.343%
9	7.684	727	731	735	rVB	18838	28203	1.05%	0.309%
10	7.872	757	763	771	rBV	30927	56861	2.12%	0.624%
11	8.107	792	803	807	rBV	67588	124704	4.65%	1.368%
12	8.154	807	811	818	rVB4	27345	55465	2.07%	0.608%
13	9.264	993	1000	1011	rVB	234914	432085	16.10%	4.739%
14	10.915	1272	1281	1287	rBV	87434	161621	6.02%	1.773%
15	11.819	1429	1435	1444	rBV3	13687	32336	1.20%	0.355%
16	13.088	1646	1651	1658	rBV2	27551	43119	1.61%	0.473%
17	13.353	1686	1696	1702	rBV	667715	1087994	40.54%	11.933%
18	13.570	1727	1733	1741	rBV	431839	671399	25.02%	7.364%
19	14.727	1924	1930	1937	rVB	163139	262952	9.80%	2.884%
20	16.067	2153	2158	2167	rVB2	27123	41909	1.56%	0.460%
21	16.213	2177	2183	2191	rBV	657162	1062974	39.61%	11.658%
22	17.470	2390	2397	2404	rBV	274401	418410	15.59%	4.589%
23	18.128	2502	2509	2513	rVB3	37558	45133	1.68%	0.495%
24	20.079	2834	2841	2848	rBV	1962566	2683494	100.00%	29.431%
25	21.753	3119	3126	3133	rBV	319229	548446	20.44%	6.015%
26	25.048	3677	3687	3698	rVB2	187676	533017	19.86%	5.846%

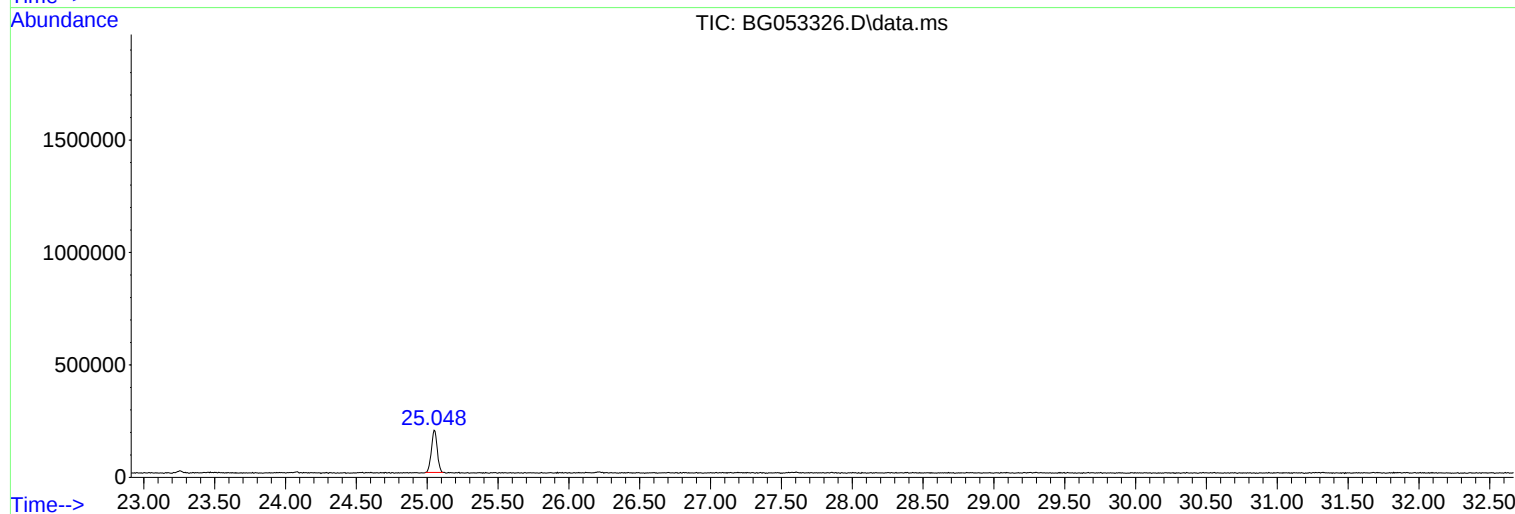
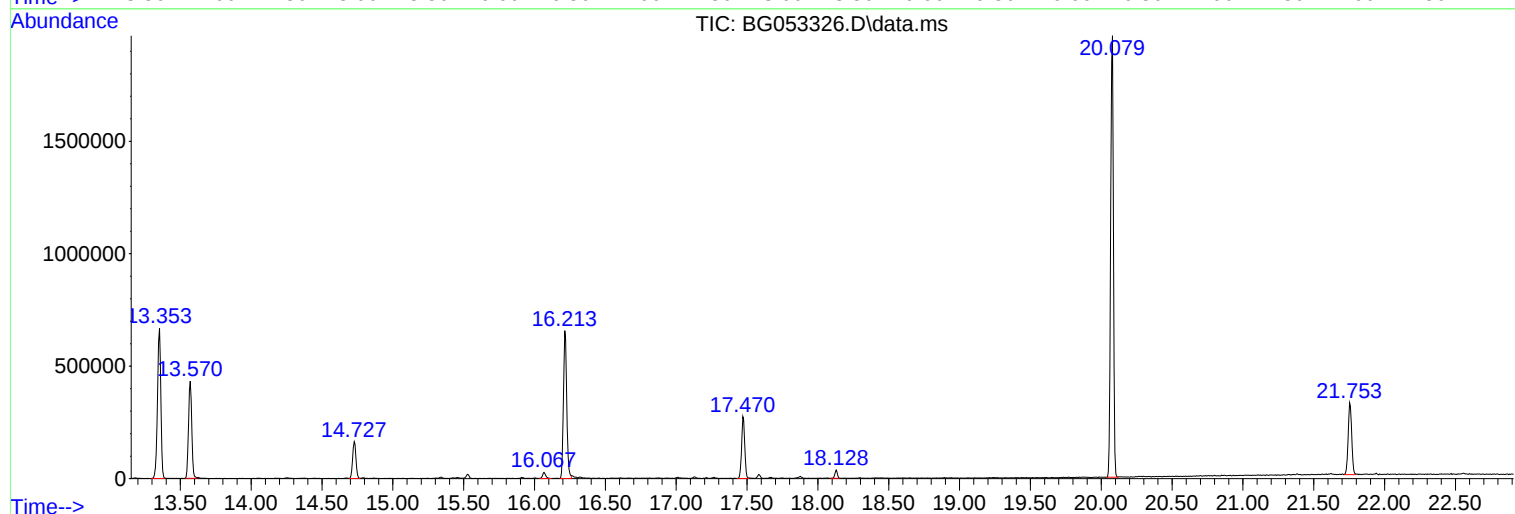
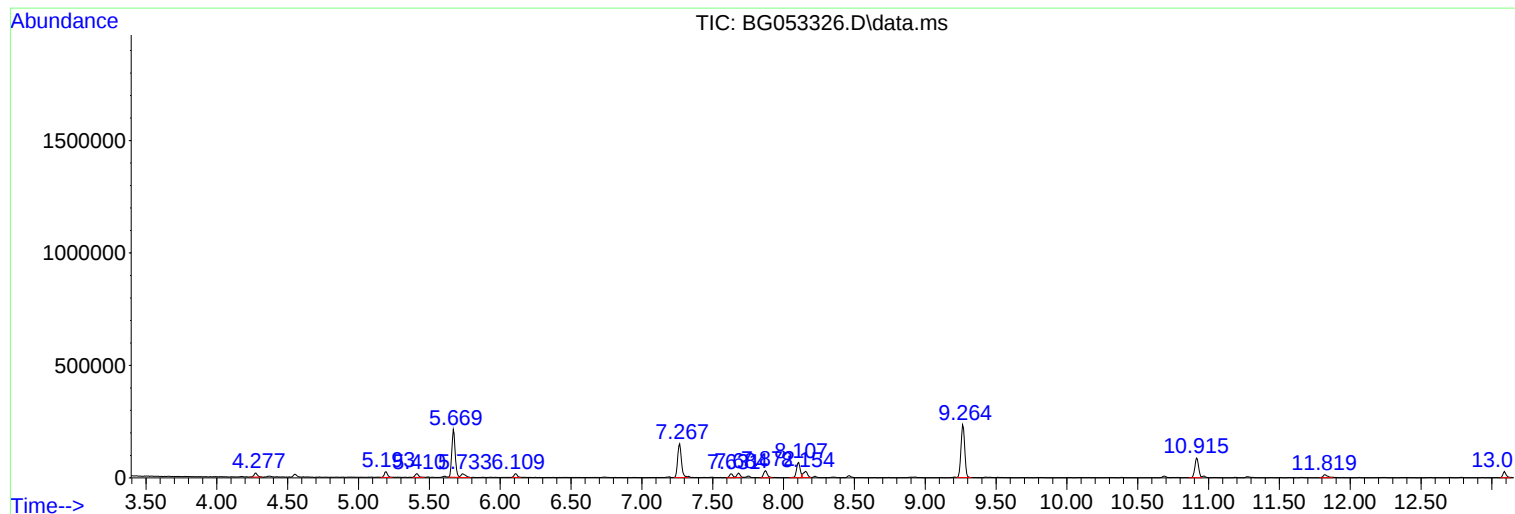
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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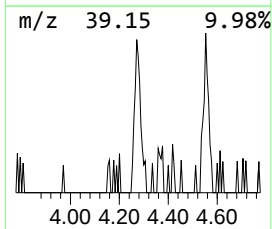
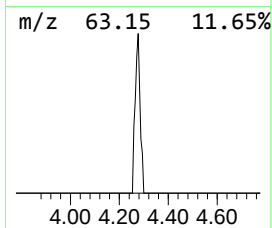
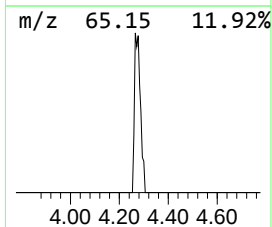
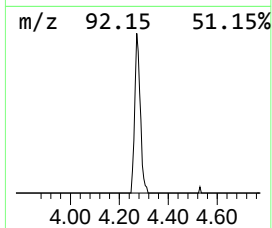
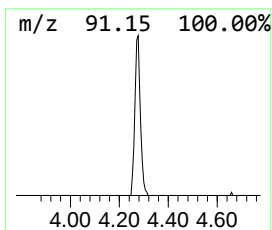
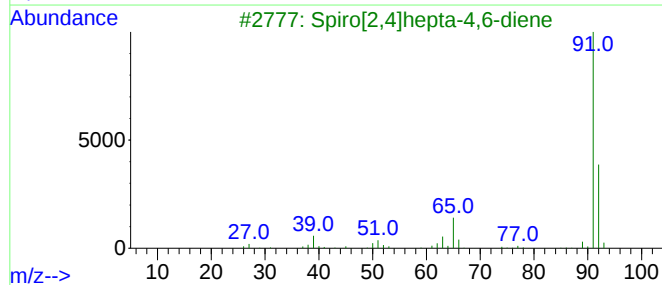
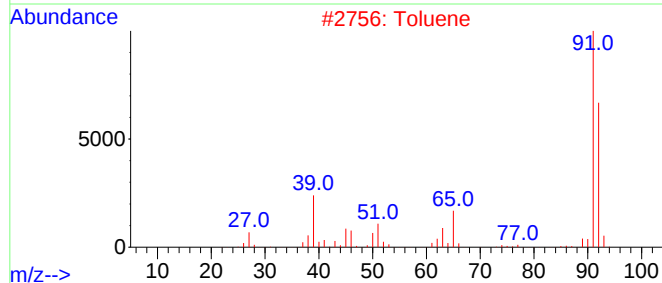
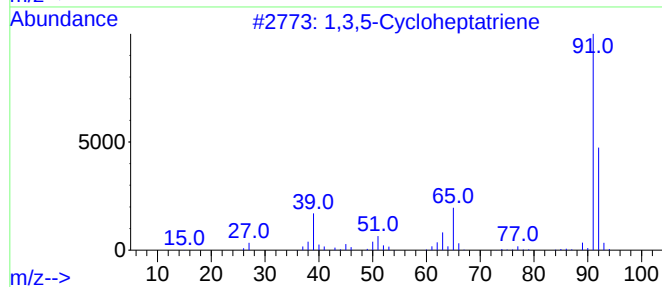
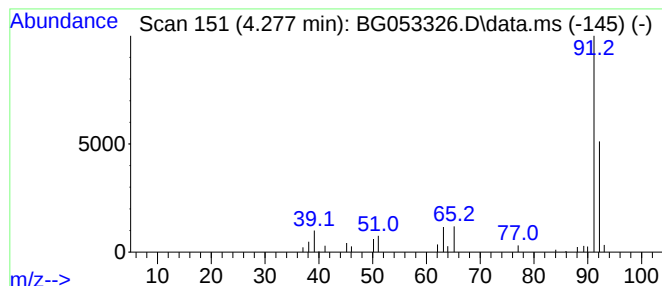
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3,5-Cycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.277	5.14 ng	32041	1,4-Dichlorobenzene-d4	8.107

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	83
2		Toluene	92	C7H8	000108-88-3	83
3		Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	80
4		Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	78
5		Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	72



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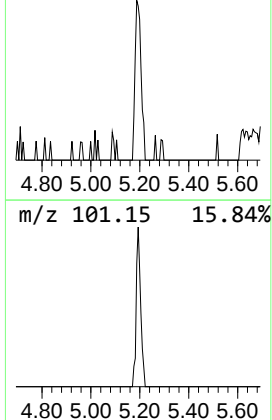
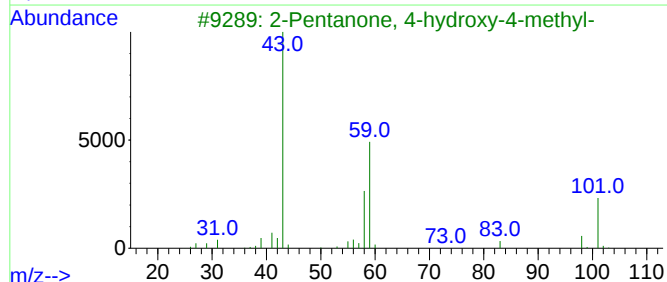
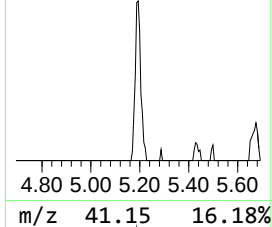
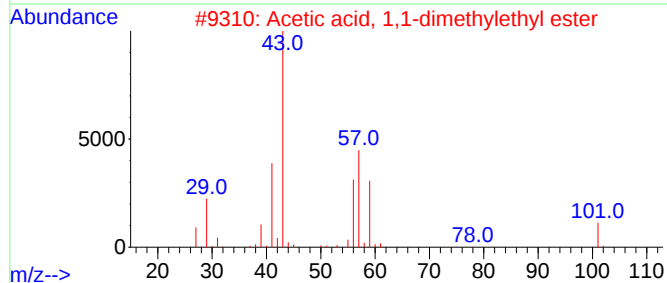
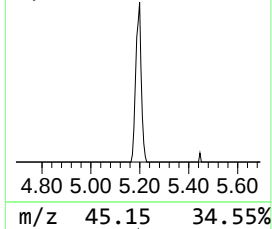
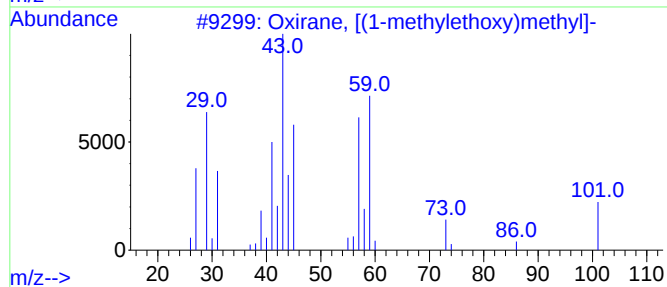
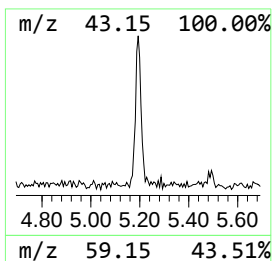
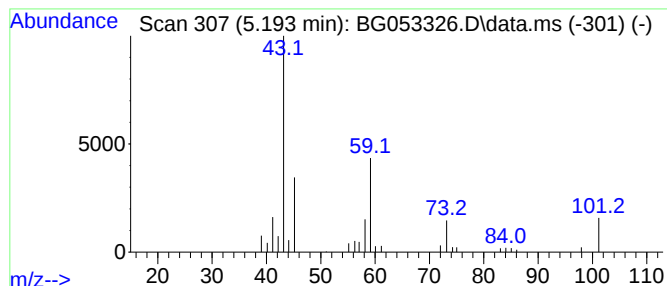
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Oxirane, [(1-methylethoxy)m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	6.77 ng	42238	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	23
4			3(2H)-Furanone, dihydro-2-methyl-	100	C5H8O2	003188-00-9	12
5			1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	12



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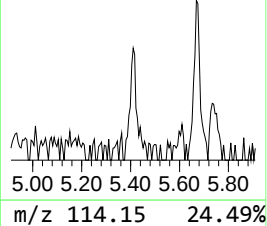
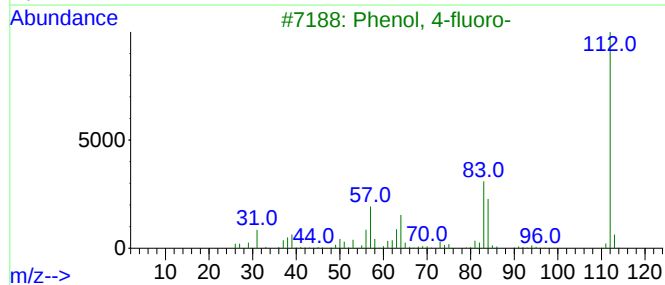
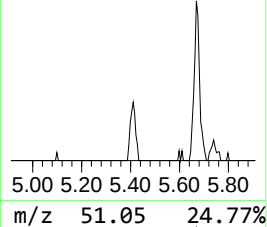
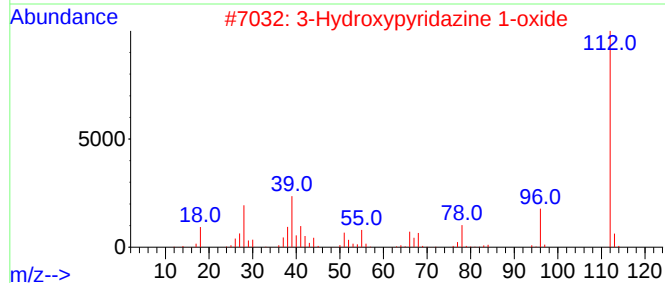
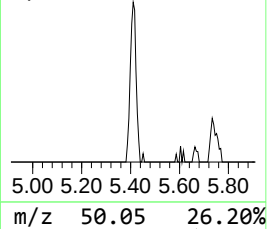
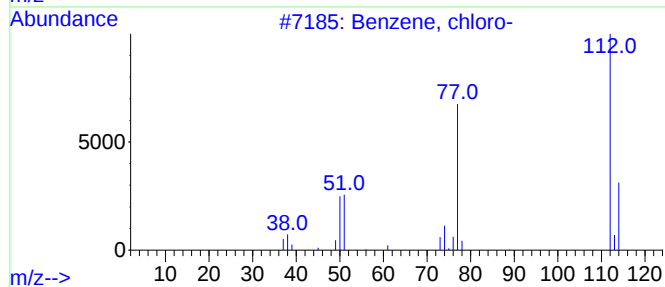
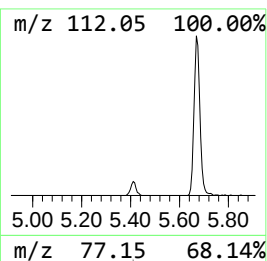
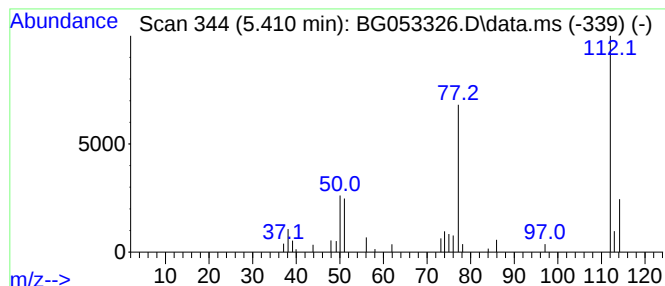
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.410	4.45 ng	27756	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, chloro-	112	C6H5Cl	000108-90-7	95
2			3-Hydroxypyridazine 1-oxide	112	C4H4N2O2	018259-51-3	35
3			Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	25
4			Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	16
5			Carbonic acid, monoamide, N-buty...	155	C8H13NO2	1000420-25-3	12



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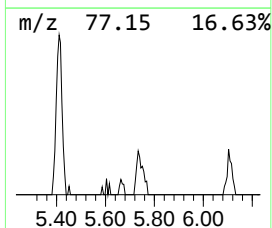
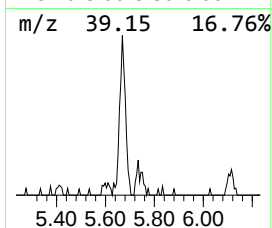
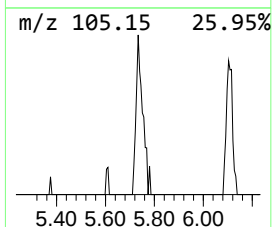
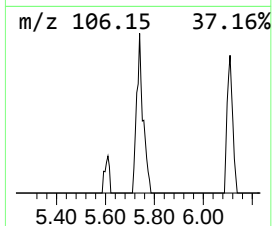
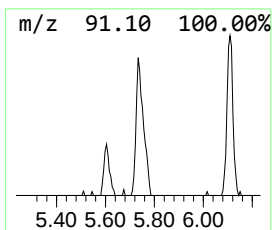
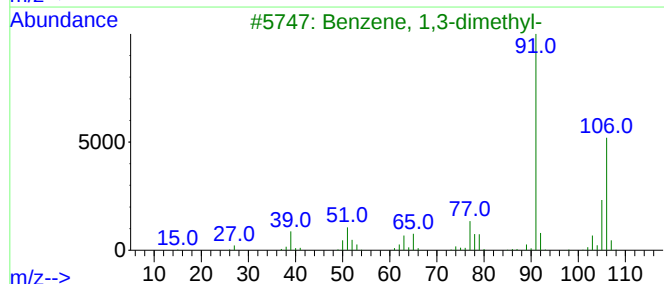
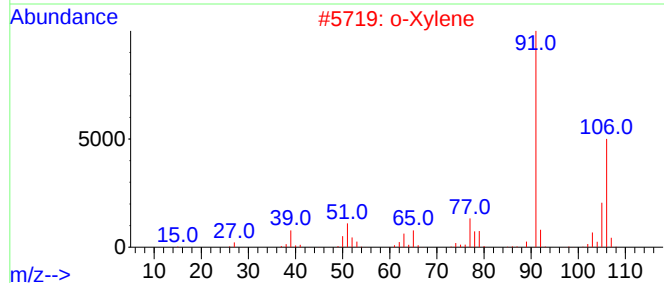
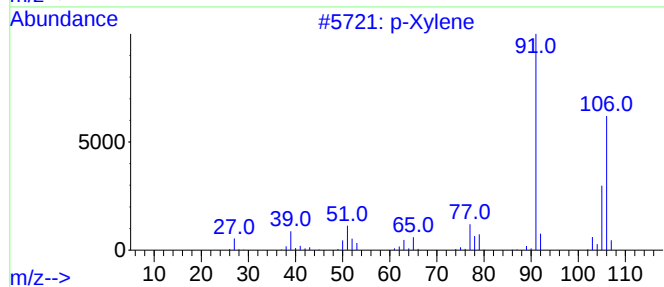
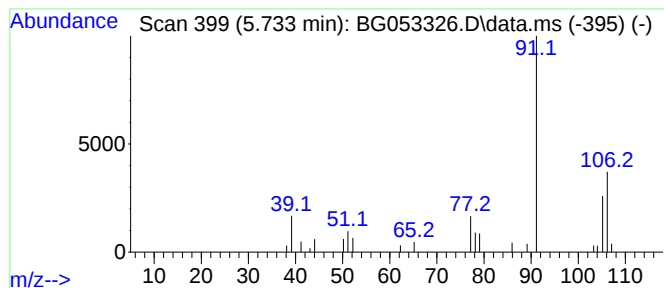
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 p-Xylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.733	6.14 ng	38255	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Xylene	106	C8H10	000106-42-3	90
2			o-Xylene	106	C8H10	000095-47-6	72
3			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	72
4			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	64
5			Ethylbenzene	106	C8H10	000100-41-4	59



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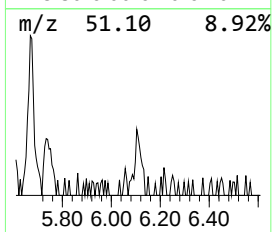
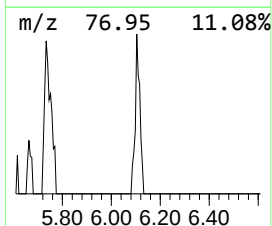
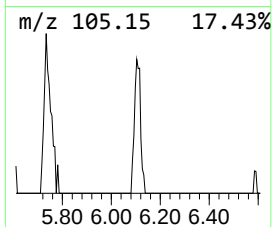
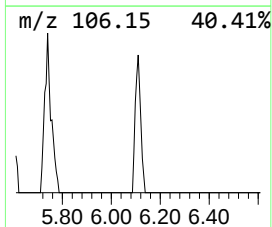
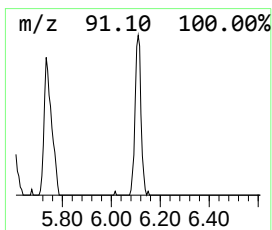
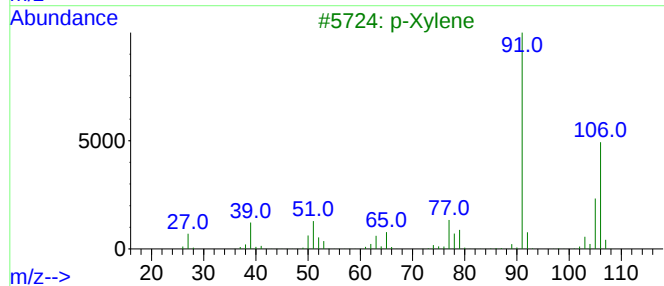
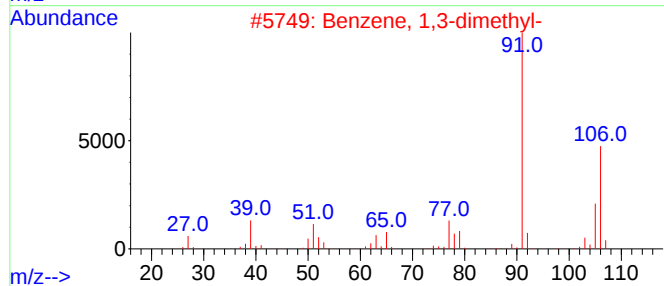
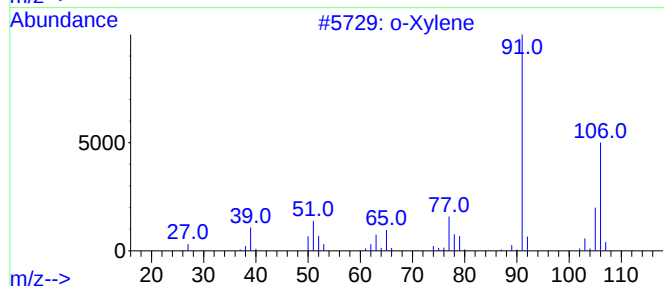
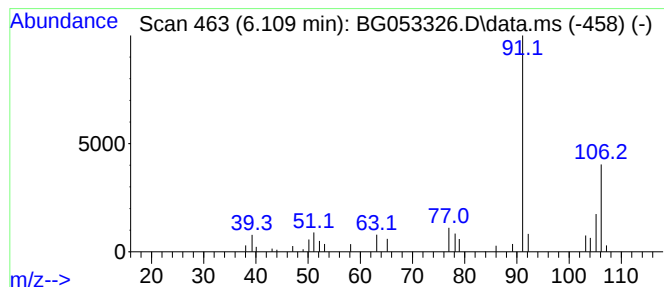
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 o-Xylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.109	4.49 ng	28016	1,4-Dichlorobenzene-d4	8.107

Hit#	of	4	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Xylene	106	C8H10	000095-47-6	90
2			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	90
3			p-Xylene	106	C8H10	000106-42-3	90
4			Ethylbenzene	106	C8H10	000100-41-4	86



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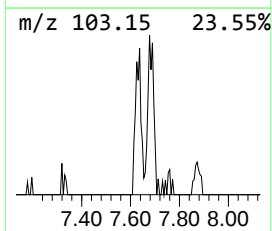
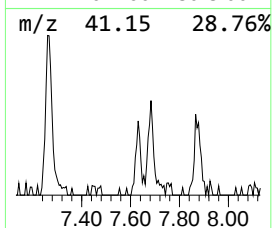
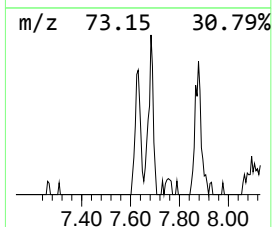
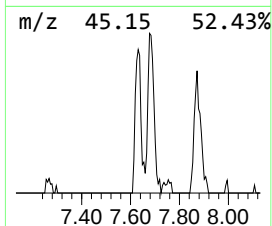
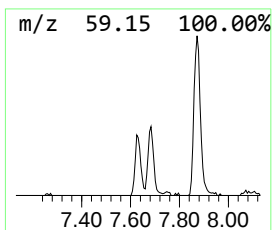
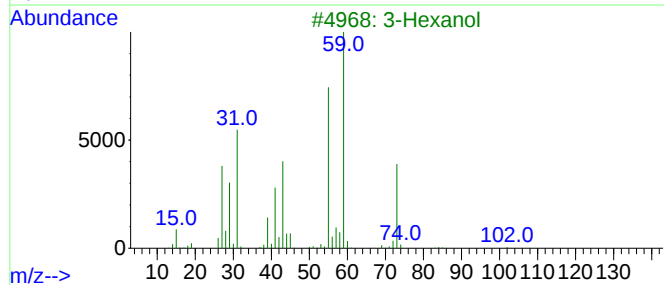
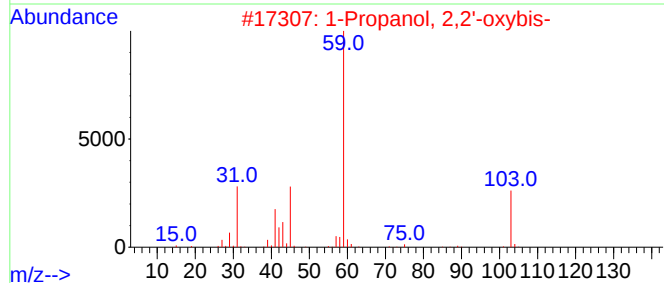
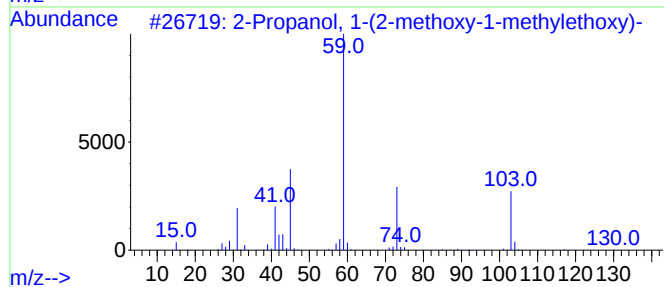
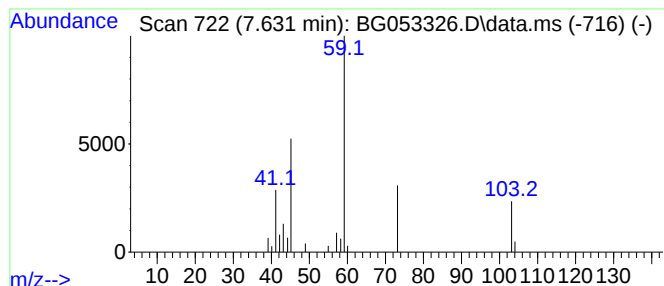
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.631	5.01 ng	31236	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	50		
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42		
3	3-Hexanol	102	C6H14O	000623-37-0	40		
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	40		
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	36		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053326.D
Acq On : 26 Apr 2022 18:52
Operator : CG/JU
Sample : N2482-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-2R

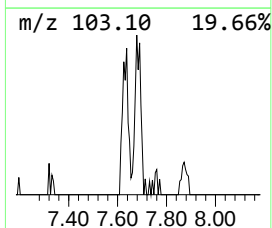
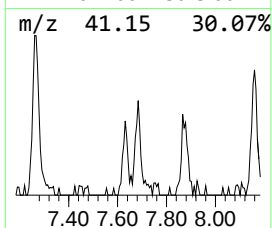
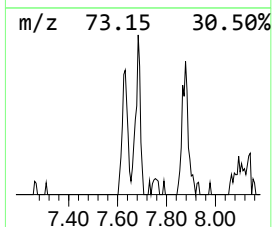
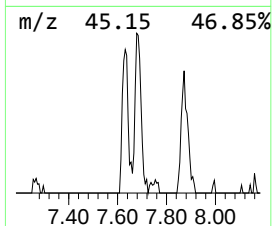
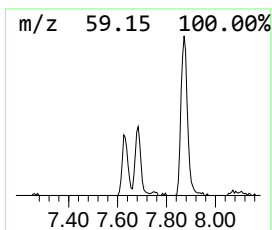
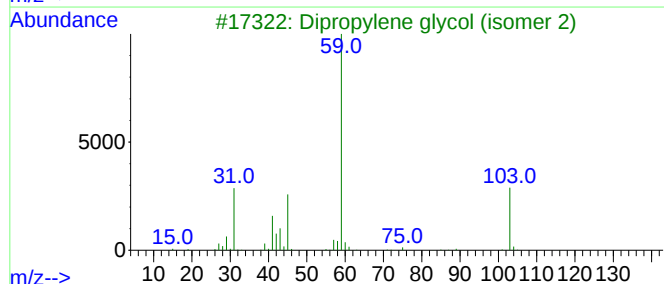
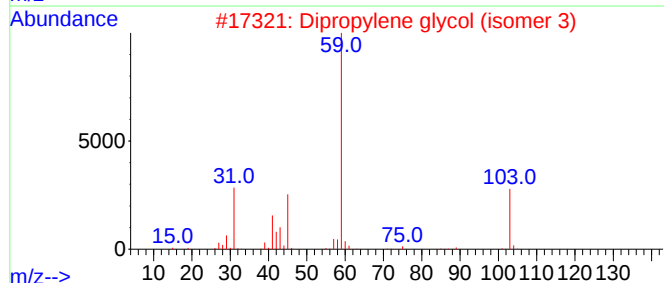
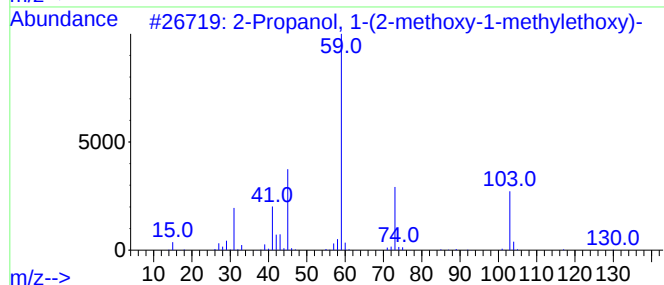
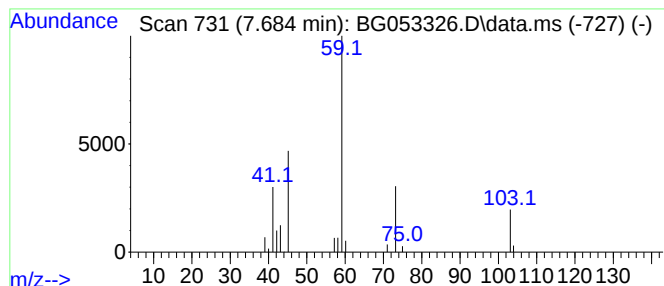
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.684 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.684	4.52 ng	28203	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74		
2	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	45		
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	45		
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	45		
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	45		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053326.D
Acq On : 26 Apr 2022 18:52
Operator : CG/JU
Sample : N2482-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-2R

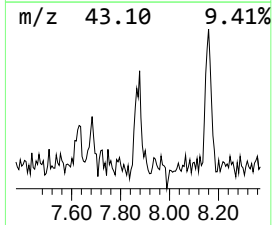
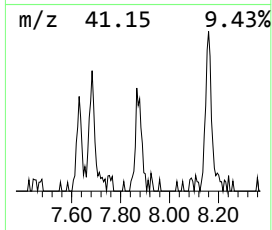
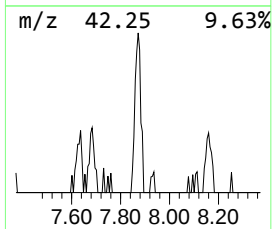
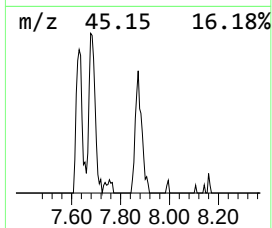
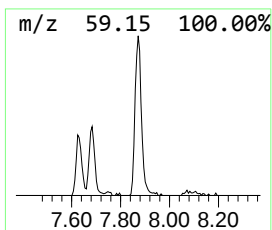
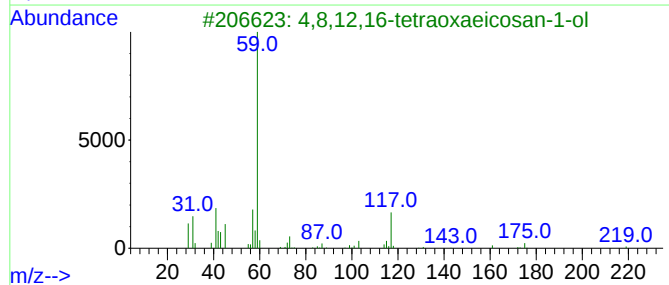
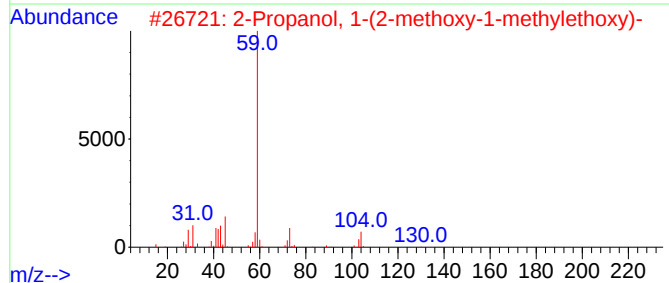
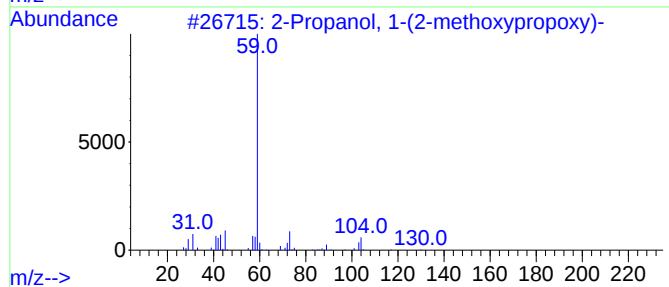
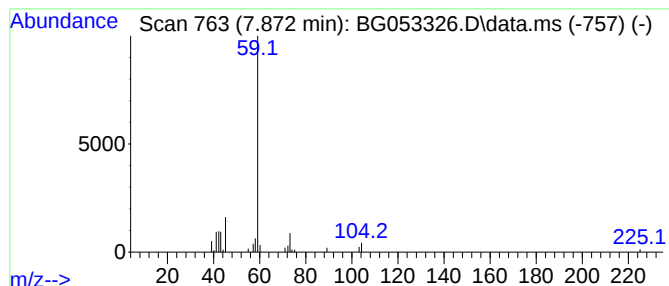
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.872	9.12 ng	56861	1,4-Dichlorobenzene-d4	8.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83		
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
3	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	72		
4	Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	64		
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053326.D
Acq On : 26 Apr 2022 18:52
Operator : CG/JU
Sample : N2482-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-2R

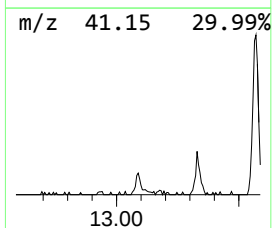
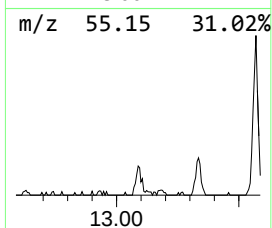
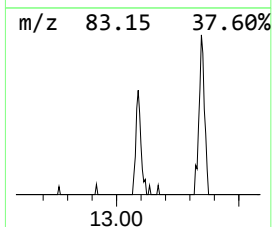
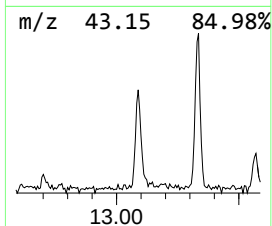
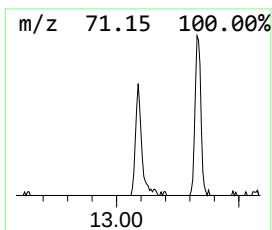
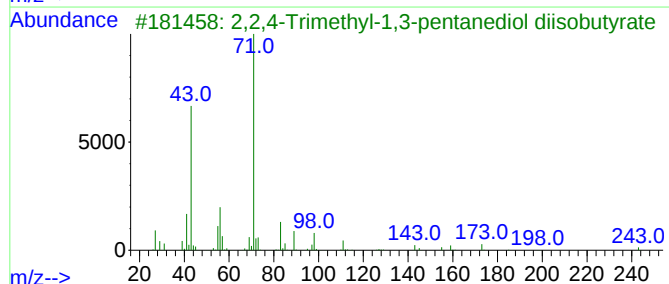
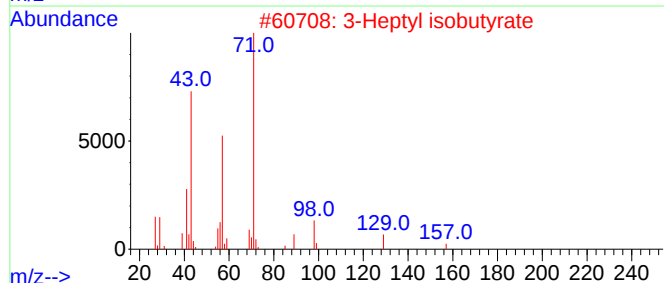
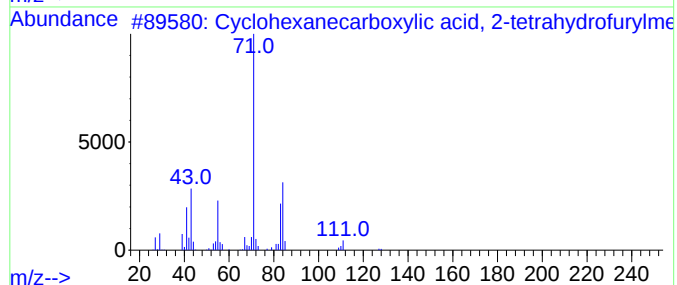
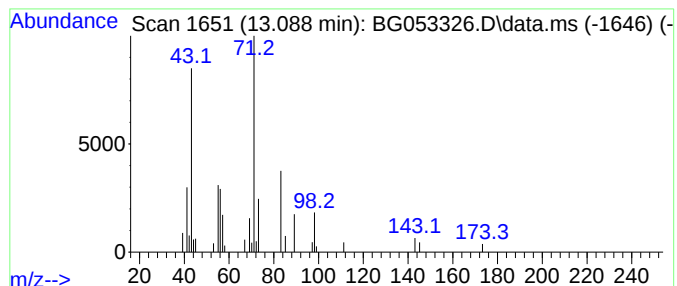
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.088 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.088	3.28 ng	43119	Acenaphthene-d10	14.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid, 2-te...	212	C12H20O3	1000279-85-7	47
2			3-Heptyl isobutyrate	186	C11H22O2	1000430-90-3	43
3			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	42
4			2-Decanol, 2-methylpropionate	228	C14H28O2	1000447-30-4	40
5			Butanoic acid, 1-methylhexyl ester	186	C11H22O2	039026-94-3	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053326.D
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Operator : CG/JU
Sample : N2482-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

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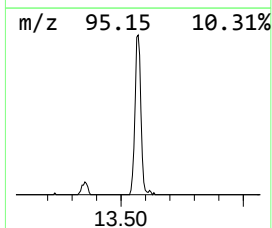
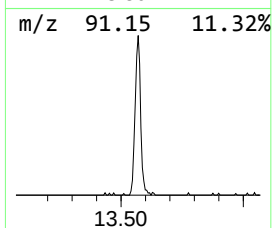
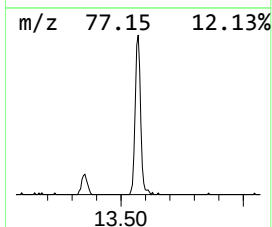
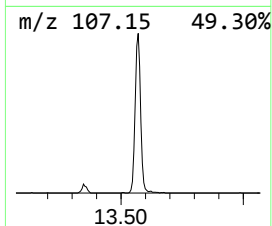
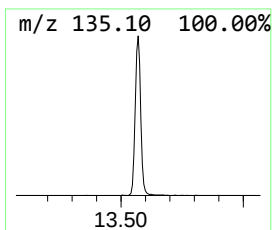
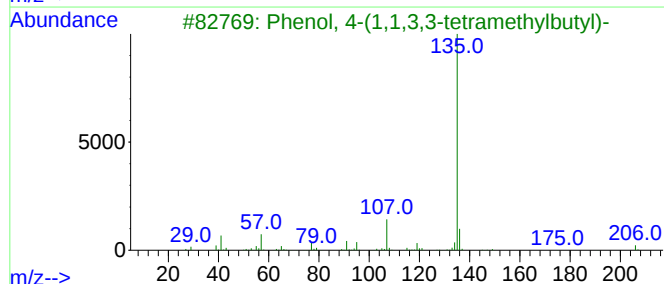
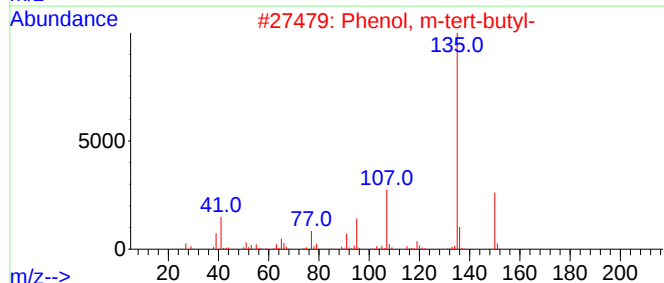
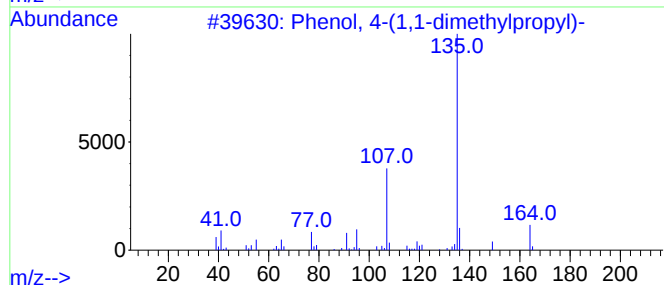
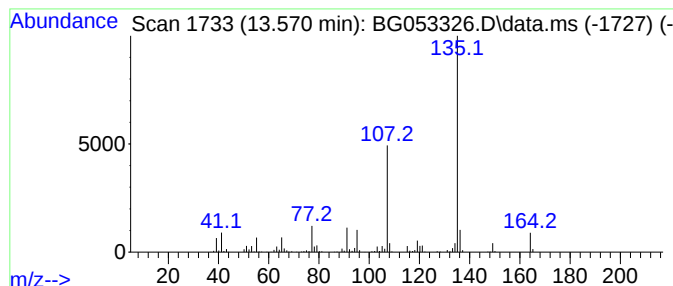
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.570	51.07 ng	671399	Acenaphthene-d10	14.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
3			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
4			Hexestrol	270	C18H22O2	000084-16-2	64
5			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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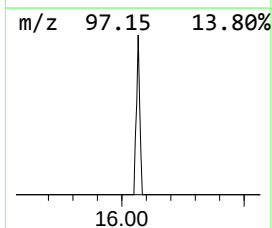
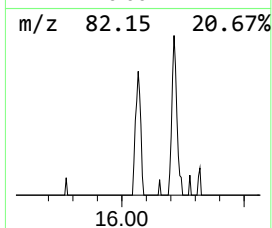
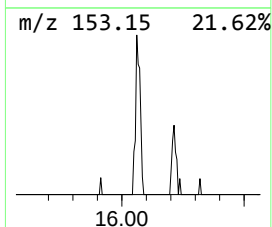
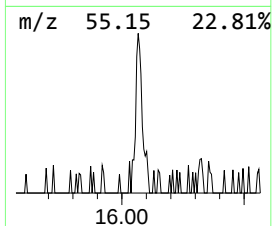
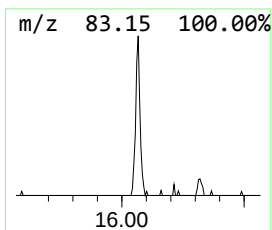
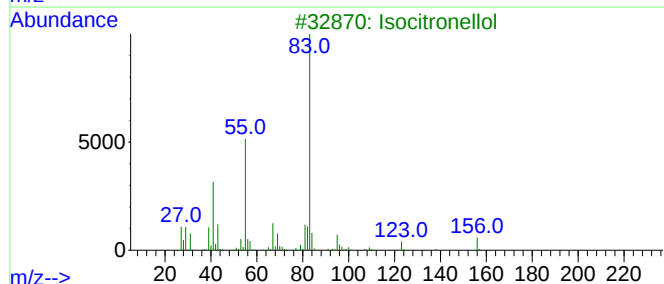
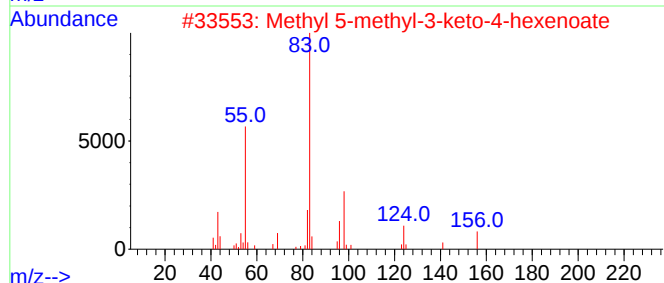
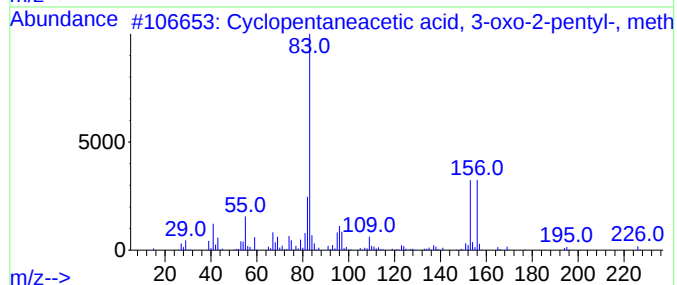
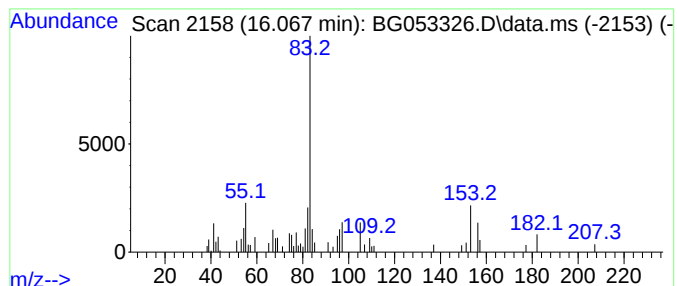
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentaneacetic acid, 3-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.067	3.19 ng	41909	Acenaphthene-d10	14.727

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	78
2			Methyl 5-methyl-3-keto-4-hexenoate	156	C8H12O3	1000427-08-8	53
3			Isocitronellol	156	C10H20O	018479-52-2	50
4			Heptylcyclohexane	182	C13H26	005617-41-4	47
5			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053326.D
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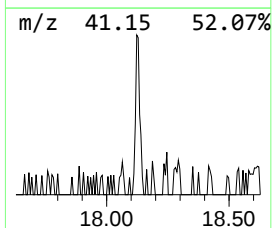
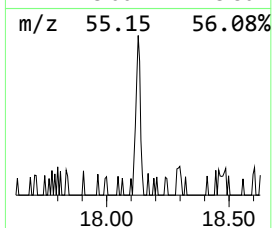
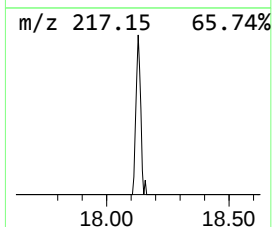
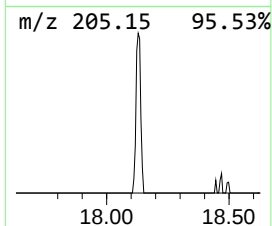
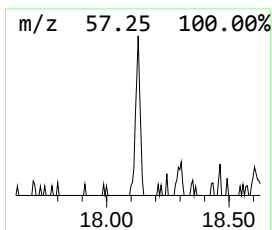
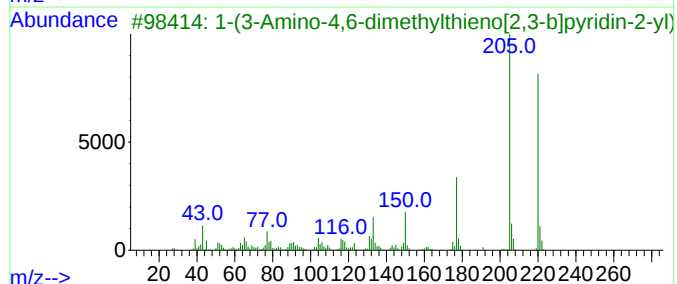
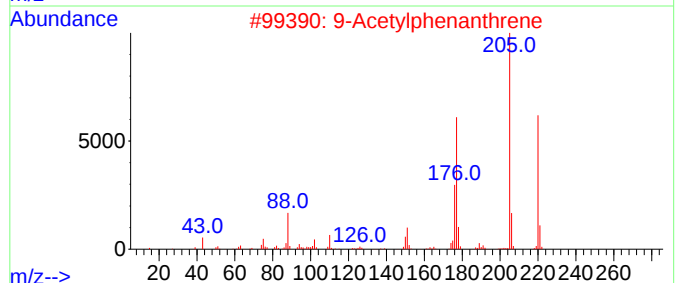
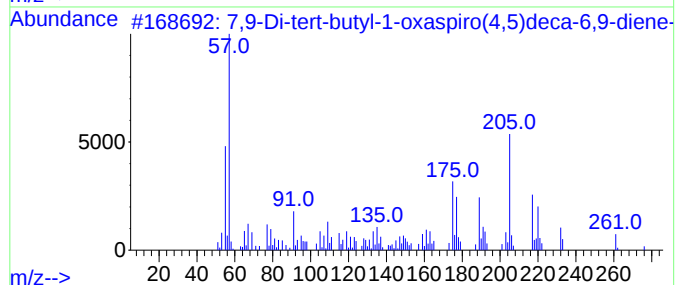
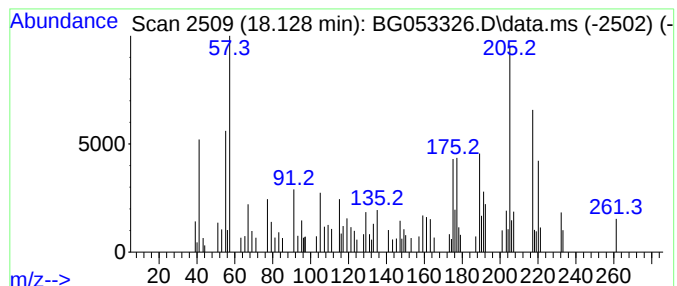
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.128	2.16 ng	45133	Phenanthrene-d10		17.471

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	91	
2	9-Acetylphenanthrene	220	C16H12O	002039-77-2	50	
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45	
4	1-Ethyl-2-methylphenanthrene	220	C17H16	061983-53-7	38	
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042622\
Data File : BG053326.D
Acq On : 26 Apr 2022 18:52
Operator : CG/JU
Sample : N2482-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COP-2R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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
1,3,5-Cyclohept...	4.277	5.1	ng	32041	1	8.107	124704	20.0
Oxirane, [(1-me...	5.193	6.8	ng	42238	1	8.107	124704	20.0
Benzene, chloro-	5.410	4.5	ng	27756	1	8.107	124704	20.0
p-Xylene	5.733	6.1	ng	38255	1	8.107	124704	20.0
o-Xylene	6.109	4.5	ng	28016	1	8.107	124704	20.0
2-Propanol, 1-(...	7.631	5.0	ng	31236	1	8.107	124704	20.0
unknown7.684	7.684	4.5	ng	28203	1	8.107	124704	20.0
2-Propanol, 1-(...	7.872	9.1	ng	56861	1	8.107	124704	20.0
unknown13.088	13.088	3.3	ng	43119	3	14.727	262952	20.0
Phenol, 4-(1,1-...	13.570	51.1	ng	671399	3	14.727	262952	20.0
Cyclopentaneace...	16.067	3.2	ng	41909	3	14.727	262952	20.0
7,9-Di-tert-but...	18.128	2.2	ng	45133	4	17.471	418410	20.0