

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
 Data File : BG049973.D
 Acq On : 25 Aug 2021 18:17
 Operator : CG/JU
 Sample : M3528-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PT-3-082421

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-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.540	419	426	436	rBV	421040	719452	61.68%	7.865%
2	6.944	656	665	671	rBV	218132	376130	32.25%	4.112%
3	6.985	671	672	678	rVV3	16841	20833	1.79%	0.228%
4	7.055	678	684	692	rVV	125096	209503	17.96%	2.290%
5	7.155	692	701	712	rVB	451562	791707	67.88%	8.655%
6	7.977	834	841	850	rVB	124522	210285	18.03%	2.299%
7	9.152	1033	1041	1051	rBV	299745	542689	46.53%	5.933%
8	10.116	1200	1205	1210	rBV4	9230	15130	1.30%	0.165%
9	10.562	1274	1281	1290	rBV2	31964	65025	5.58%	0.711%
10	10.803	1313	1322	1329	rBV	163238	303323	26.01%	3.316%
11	13.253	1732	1739	1748	rBV	749598	1166336	100.00%	12.750%
12	14.028	1866	1871	1881	rVB	66805	102763	8.81%	1.123%
13	14.639	1965	1975	1981	rBV	251809	396383	33.99%	4.333%
14	14.974	2027	2032	2038	rVB	11353	18542	1.59%	0.203%
15	15.890	2181	2188	2194	rBV2	21559	35945	3.08%	0.393%
16	16.137	2223	2230	2237	rBV	629002	990808	84.95%	10.831%
17	16.354	2261	2267	2272	rBV	40322	62806	5.38%	0.687%
18	16.607	2304	2310	2316	rBV2	52808	78169	6.70%	0.855%
19	16.871	2347	2355	2360	rBV9	18596	48458	4.15%	0.530%
20	17.394	2435	2444	2450	rBV	268280	431230	36.97%	4.714%
21	17.500	2459	2462	2465	rBV4	16143	22189	1.90%	0.243%
22	17.523	2465	2466	2470	rVB4	16592	11727	1.01%	0.128%
23	17.993	2539	2546	2552	rBV	77255	174739	14.98%	1.910%
24	18.410	2613	2617	2621	rBV6	13148	28404	2.44%	0.311%
25	19.450	2790	2794	2798	rBV	47289	69994	6.00%	0.765%
26	19.809	2852	2855	2862	rVB2	65842	95787	8.21%	1.047%
27	19.973	2879	2883	2884	rBV	90543	99223	8.51%	1.085%
28	20.002	2884	2888	2893	rVB	903258	1147220	98.36%	12.541%
29	20.367	2947	2950	2953	rBV2	50638	65998	5.66%	0.721%
30	21.671	3167	3172	3177	rVB	225934	380837	32.65%	4.163%
31	24.907	3716	3723	3733	rBV2	162140	466047	39.96%	5.095%

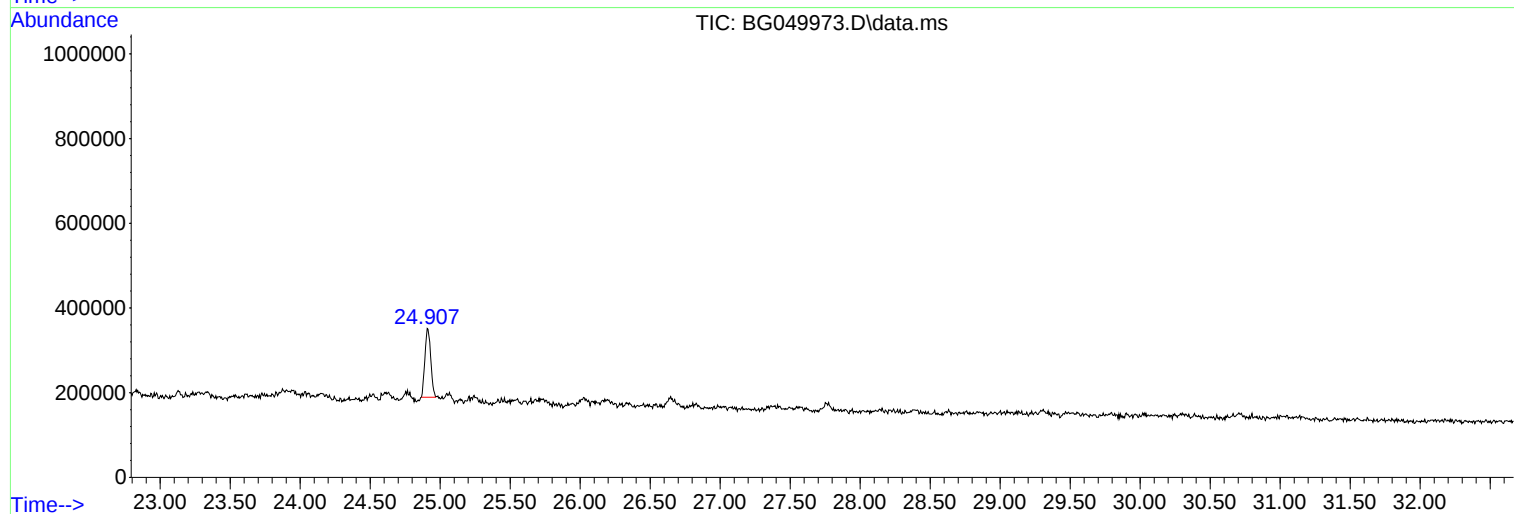
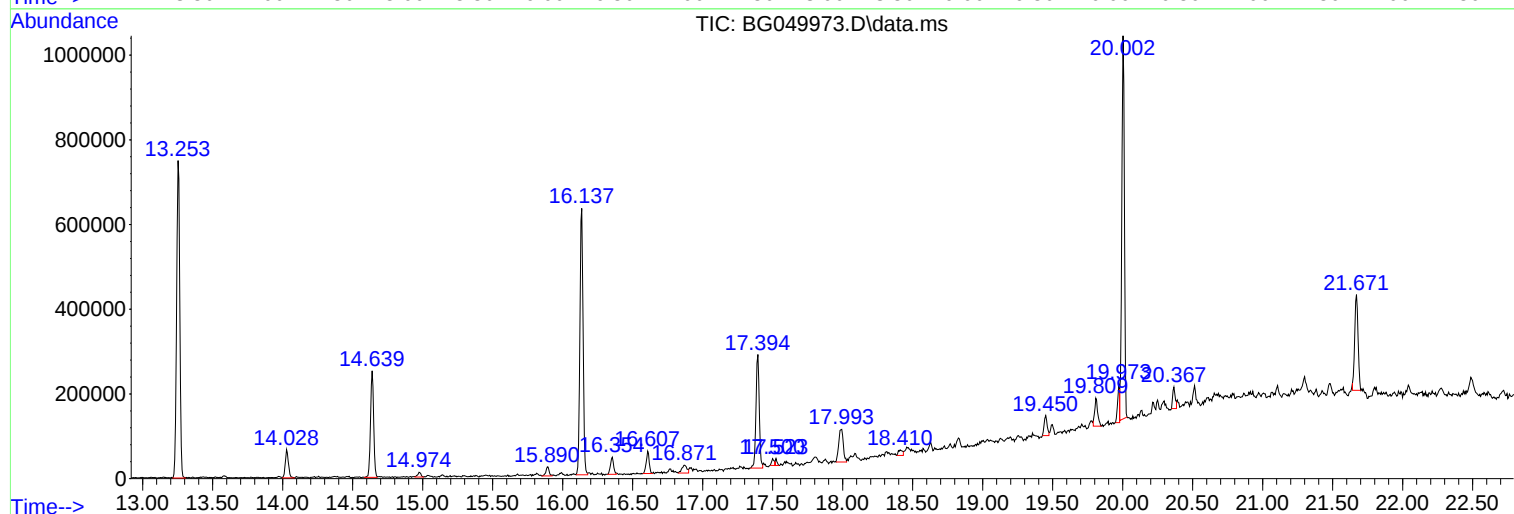
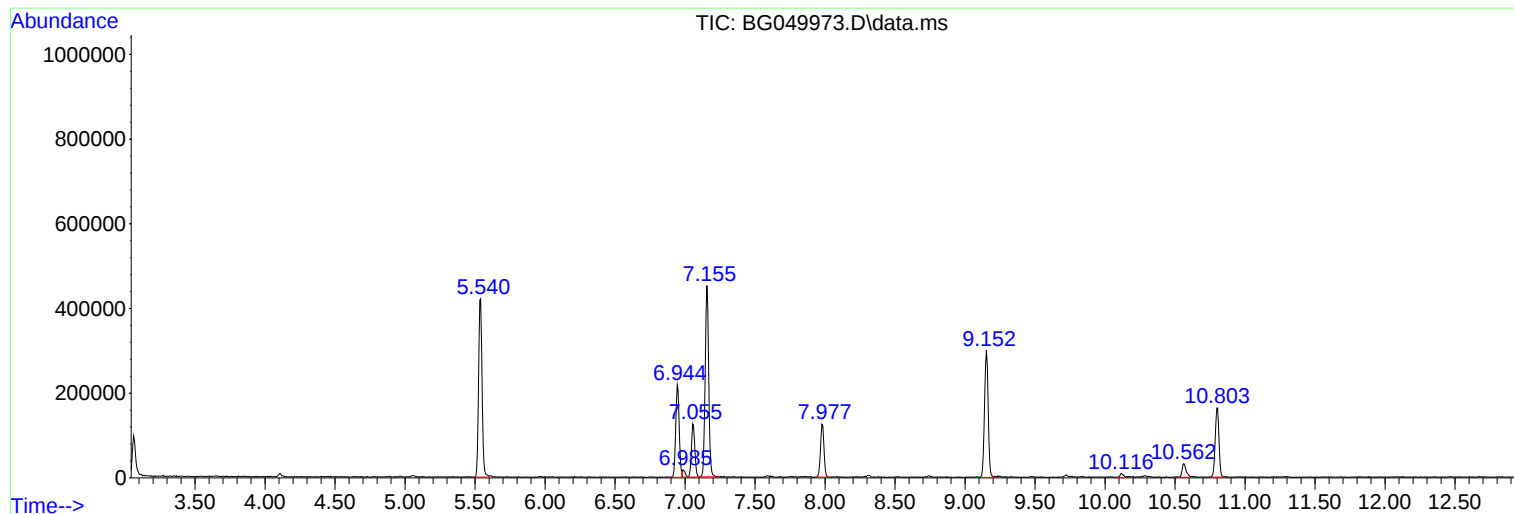
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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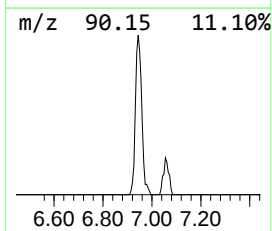
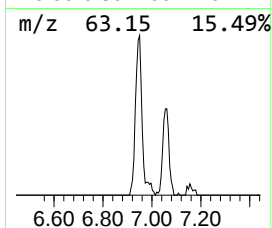
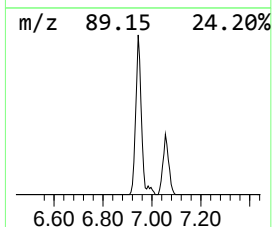
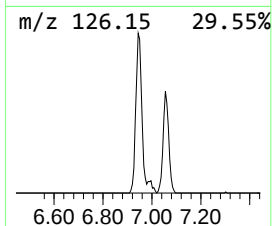
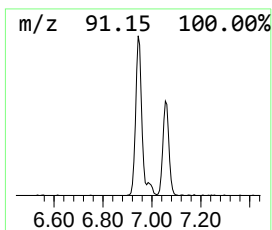
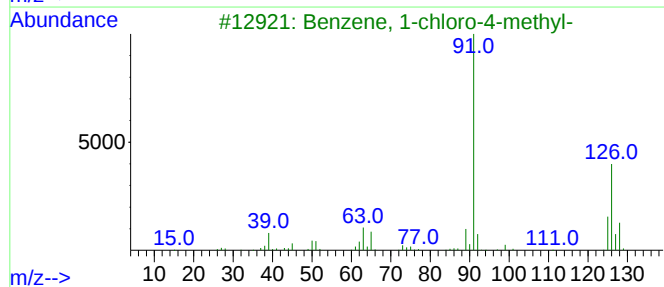
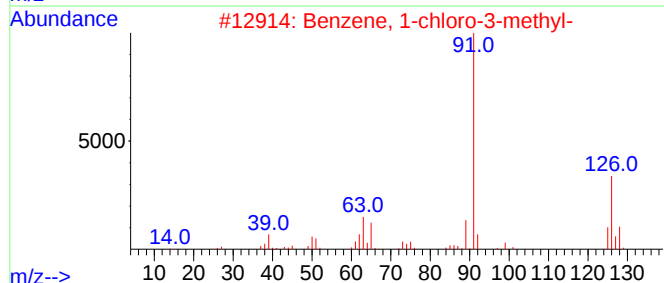
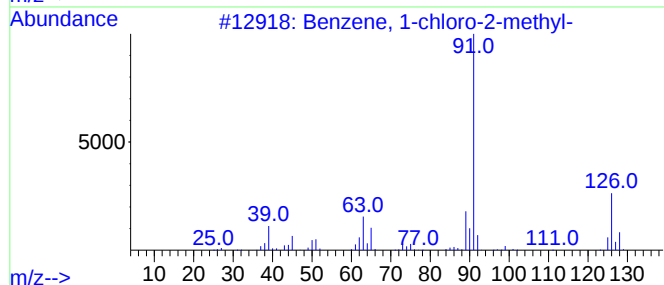
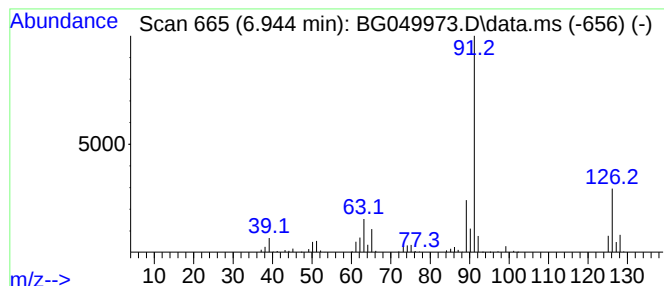
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzene, 1-chloro-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.944	35.77 ng	376130	1,4-Dichlorobenzene-d4	7.983

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	96
2			Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	95
3			Benzene, 1-chloro-4-methyl-	126	C7H7Cl	000106-43-4	76
4			Benzyl chloride	126	C7H7Cl	000100-44-7	64
5			1,6-Heptadiyne	92	C7H8	002396-63-6	22



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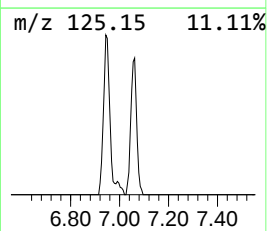
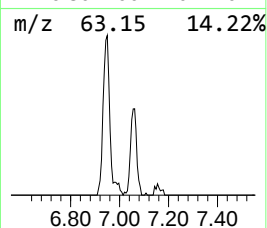
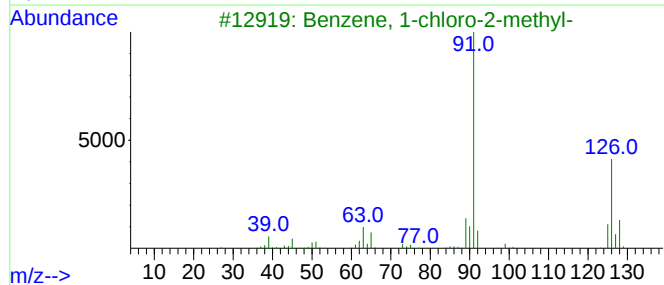
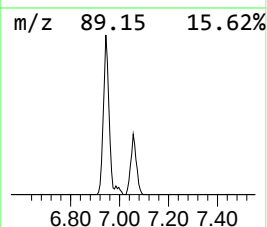
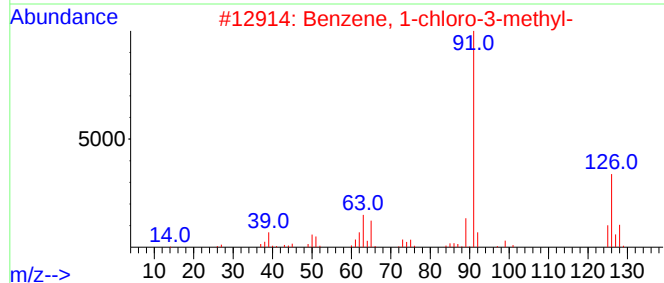
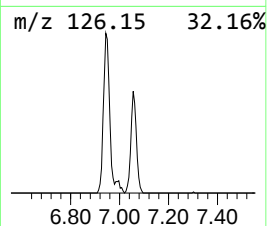
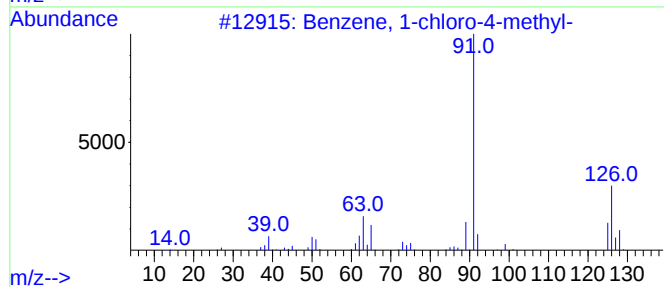
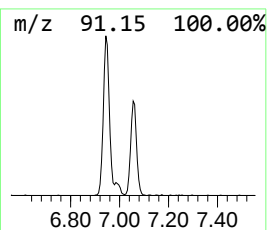
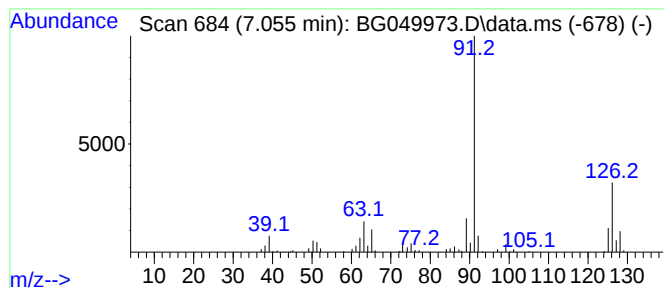
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzene, 1-chloro-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.055	19.93 ng	209503	1,4-Dichlorobenzene-d4	7.983

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-methyl-	126	C7H7Cl	000106-43-4	96
2			Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	96
3			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94
4			Benzyl chloride	126	C7H7Cl	000100-44-7	87
5			2-(p-Chlorophenyl)ethylamine	155	C8H10ClN	000156-41-2	32



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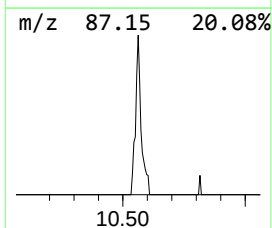
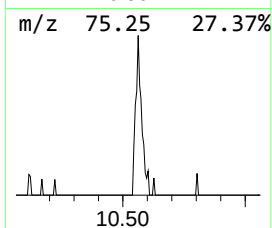
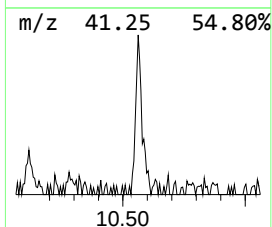
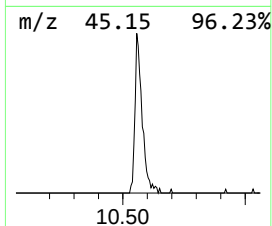
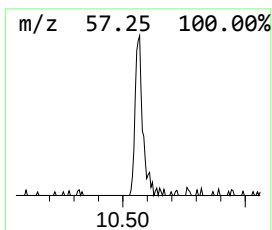
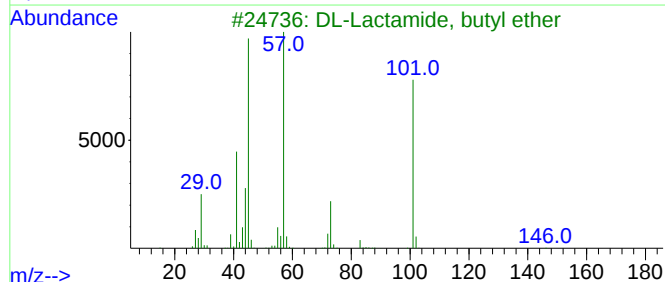
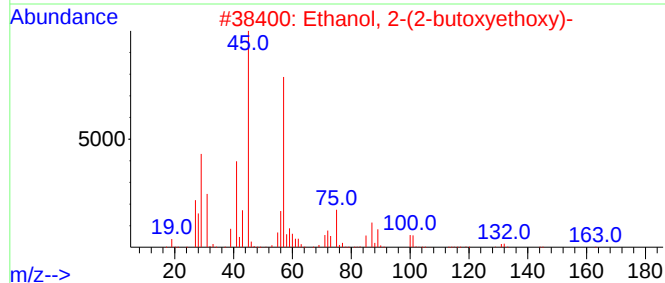
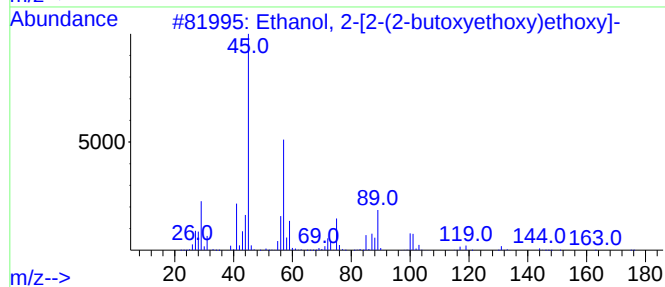
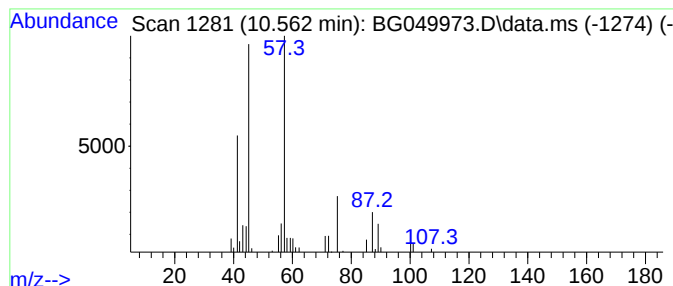
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Peak Number 3 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.562	4.29 ng	65025	Naphthalene-d8	10.803

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	50
3			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
4			Ethanol, 2-[2-(ethenyloxy)ethoxy]-	132	C6H12O3	000929-37-3	47
5			2-Propanol, 1,3-dimethoxy-	120	C5H12O3	000623-69-8	47



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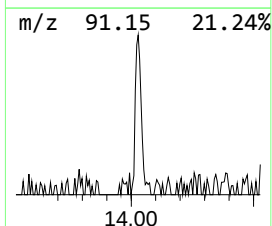
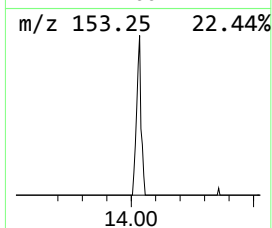
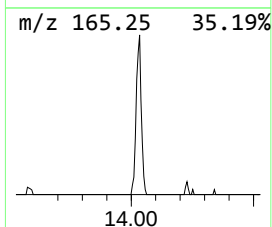
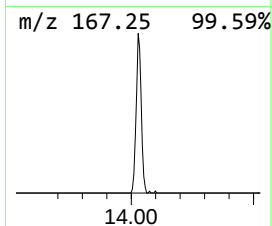
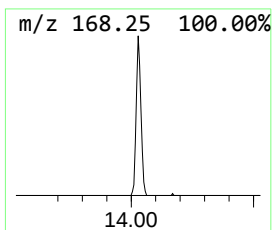
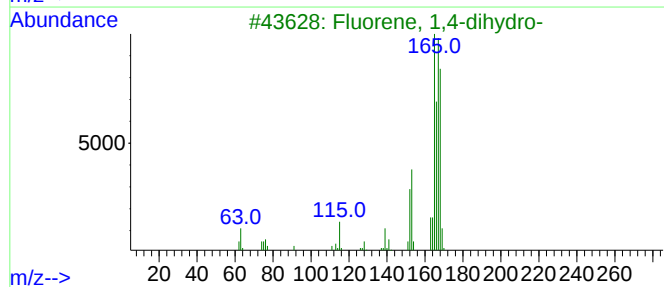
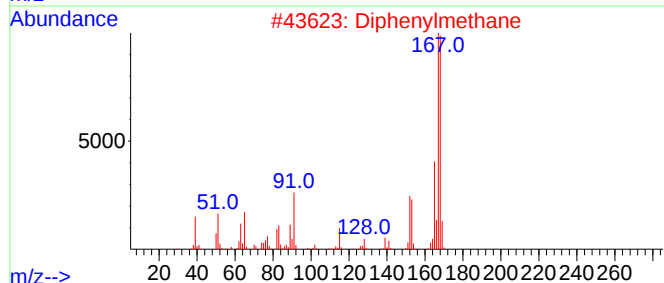
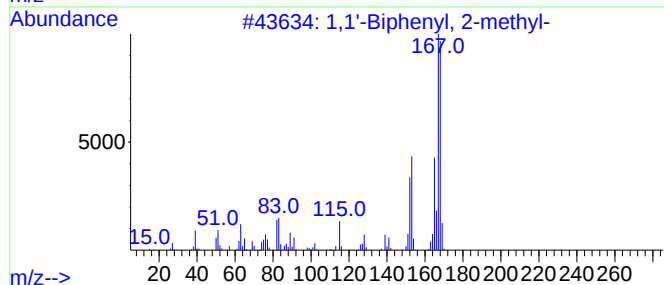
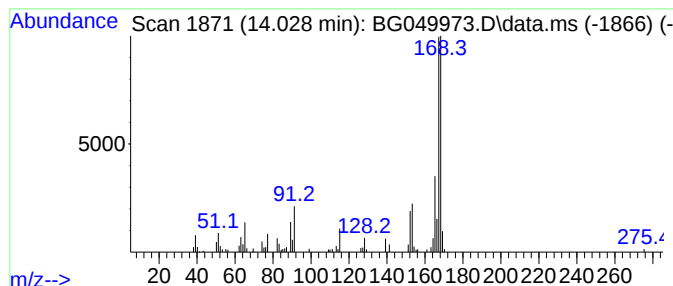
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Peak Number 4 1,1'-Biphenyl, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.028	5.19 ng	102763	Acenaphthene-d10	14.639

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	93
2		Diphenylmethane	168	C13H12	000101-81-5	93
3		Fluorene, 1,4-dihydro-	168	C13H12	041593-21-9	81
4		1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	59
5		1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	52



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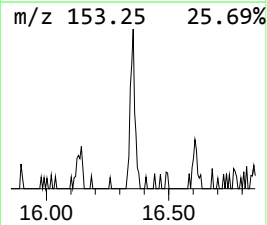
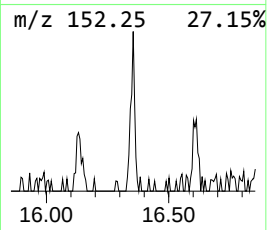
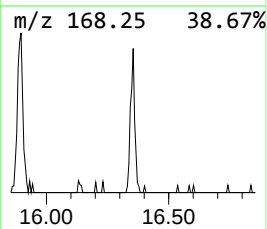
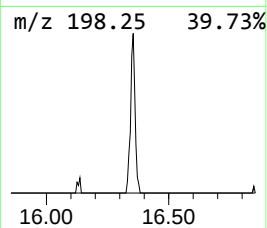
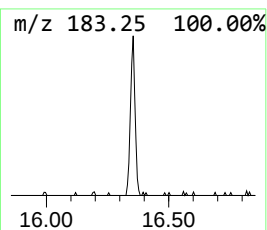
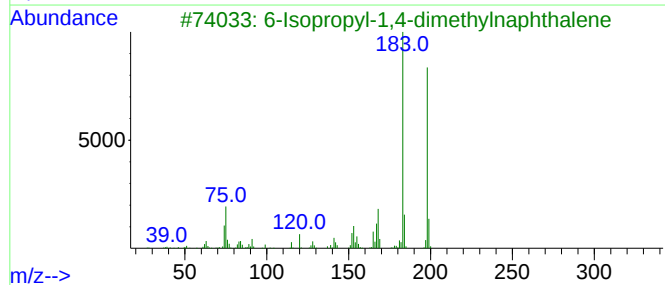
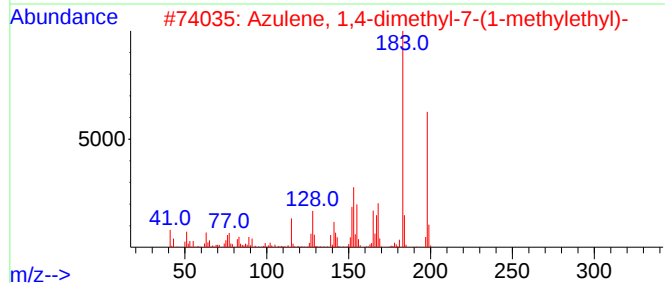
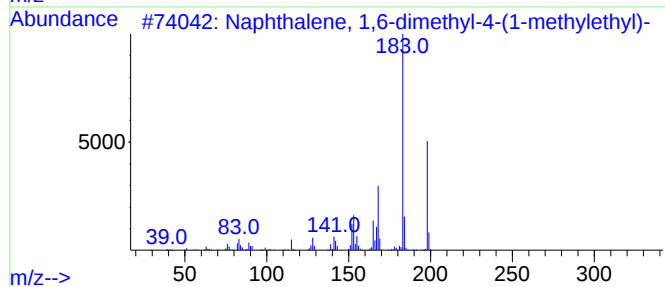
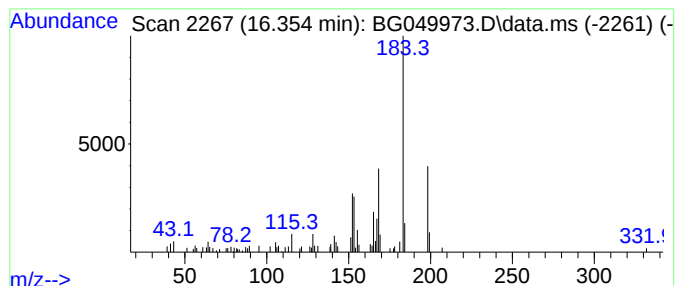
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Peak Number 5 Naphthalene, 1,6-dimethyl-4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	2.91 ng	62806	Phenanthrene-d10	17.394

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	95
2			Azulene, 1,4-dimethyl-7-(1-methy...	198	C15H18	000489-84-9	90
3			6-Isopropyl-1,4-dimethylnaphthalene	198	C15H18	000489-77-0	81
4			Phenol, 4-(1-phenylethyl)-	198	C14H14O	001988-89-2	47
5			Phloroglucinol, trimethylsilyl e...	198	C9H14O3Si	134273-02-2	47



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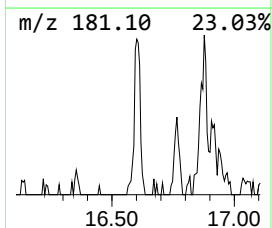
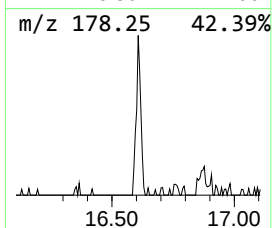
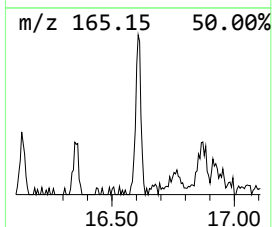
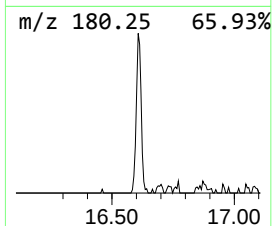
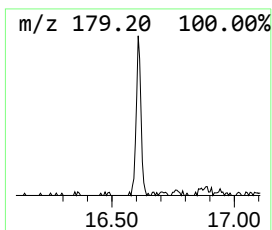
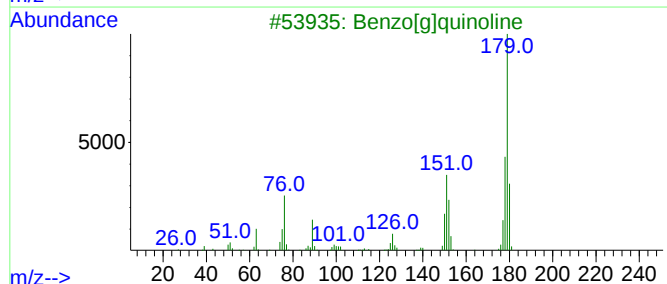
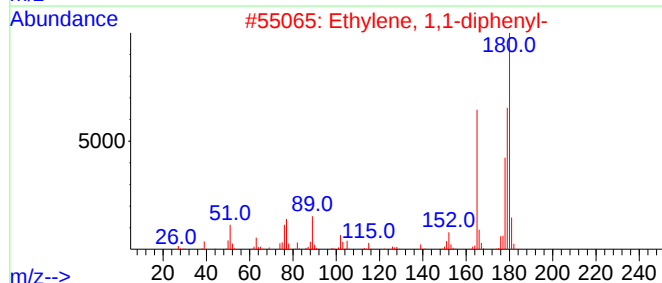
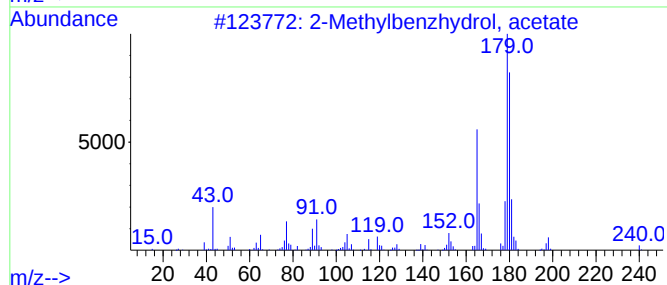
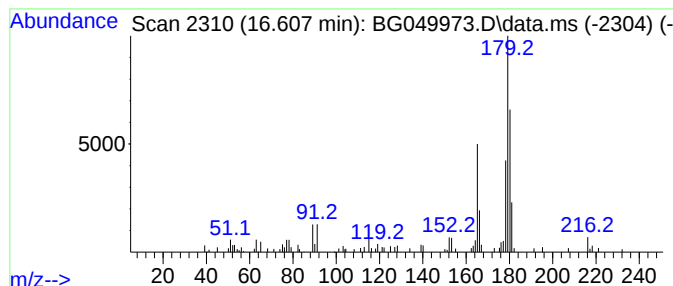
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Methylbenzhydrol, acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.607	3.63 ng	78169	Phenanthrene-d10	17.394

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylbenzhydrol, acetate	240	C16H16O2	959217-47-1	64
2		Ethylene, 1,1-diphenyl-	180	C14H12	000530-48-3	46
3		Benzo[g]quinoline	179	C13H9N	000260-36-6	43
4		Benzo[h]quinoline	179	C13H9N	000230-27-3	43
5		9H-Fluorene, 2-methyl-	180	C14H12	001430-97-3	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049973.D
Acq On : 25 Aug 2021 18:17
Operator : CG/JU
Sample : M3528-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-3-082421

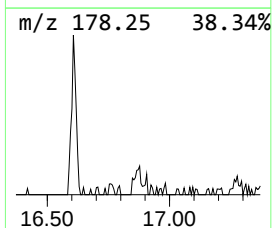
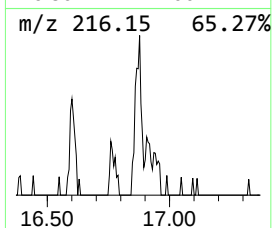
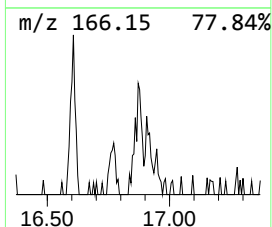
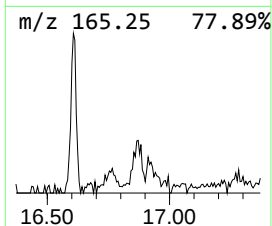
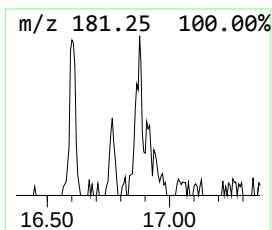
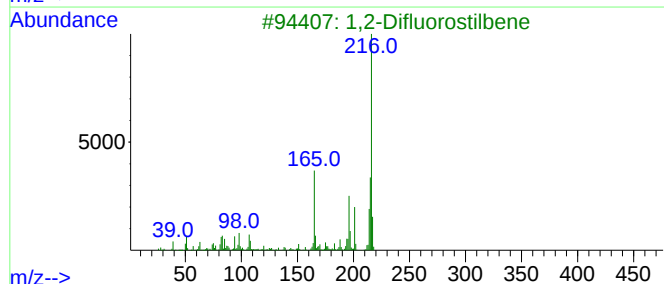
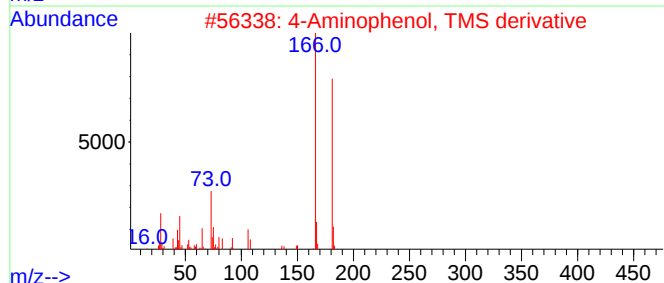
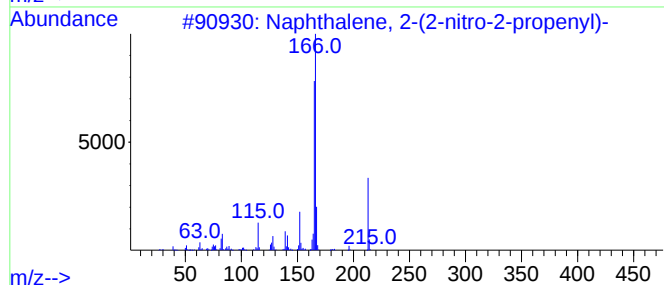
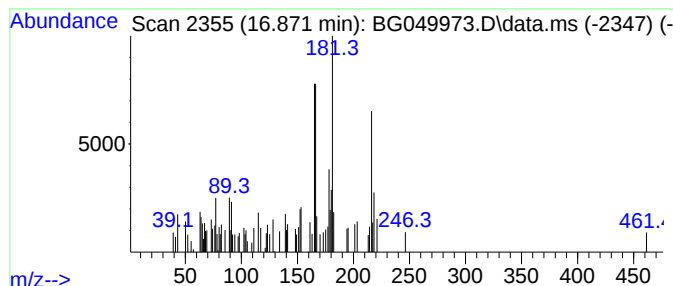
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.871 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.871	2.25 ng	48458	Phenanthrene-d10	17.394

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-(2-nitro-2-propen...	213	C13H11NO2	080255-28-3	38
2			4-Aminophenol, TMS derivative	181	C9H15NOSi	036309-42-9	30
3			1,2-Difluorostilbene	216	C14H10F2	000643-76-5	30
4			9-Amino-6-[methylthio]-9H-purine	181	C6H7N5S	020914-61-8	30
5			[1,1'-Biphenyl]-4-carbonyl chloride	216	C13H9ClO	014002-51-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049973.D
Acq On : 25 Aug 2021 18:17
Operator : CG/JU
Sample : M3528-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

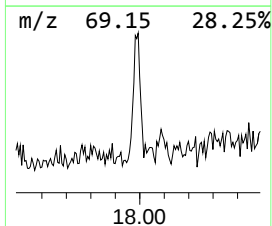
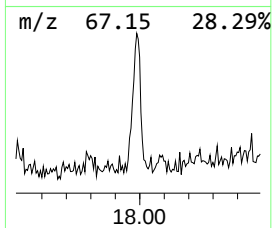
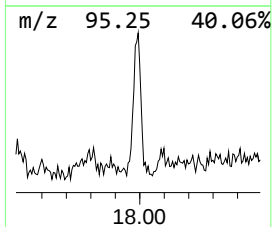
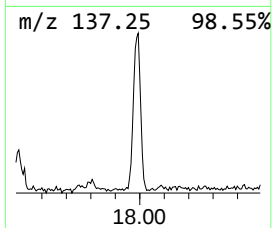
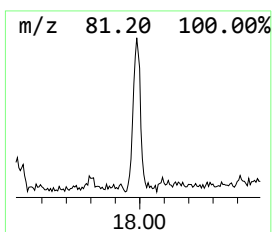
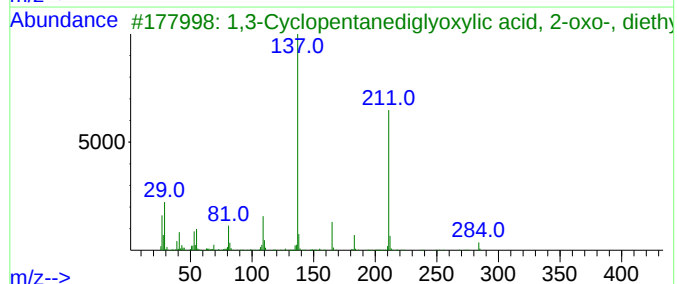
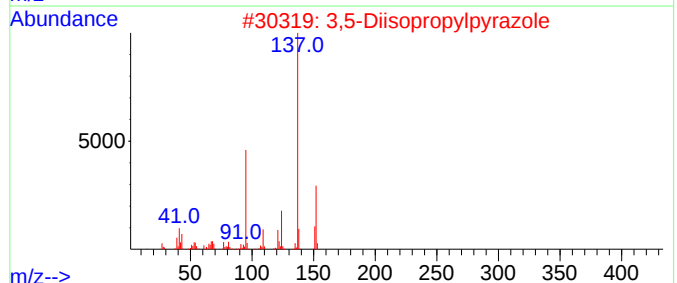
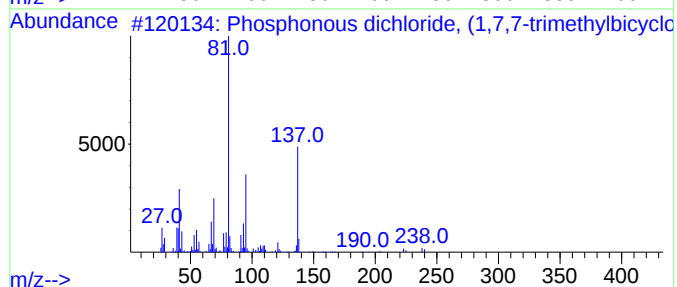
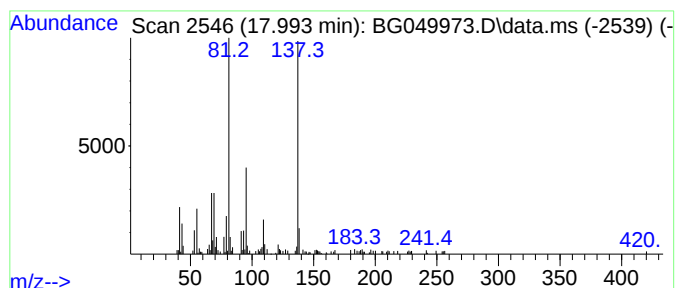
Instrument :
BNA_G
ClientSampleId :
PT-3-082421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phosphonous dichloride, (1,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.993	8.10 ng	174739	Phenanthrene-d10	17.394	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphonous dichloride, (1,7,7-t...	238	C10H17Cl2P	074630-16-3	53
2	3,5-Diisopropylpyrazole	152	C9H16N2	017536-00-4	43
3	1,3-Cyclopentanediglyoxylic acid...	284	C13H16O7	022358-21-0	35
4	4-Fluorophenyl isocyanate	137	C7H4FN0	001195-45-5	27
5	(4-Methoxy-phenyl)-(2-nitrocyclo...	265	C14H19NO4	103077-68-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049973.D
Acq On : 25 Aug 2021 18:17
Operator : CG/JU
Sample : M3528-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

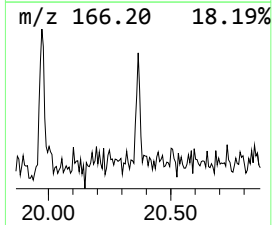
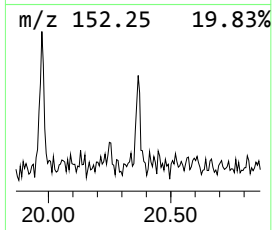
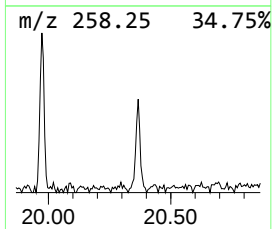
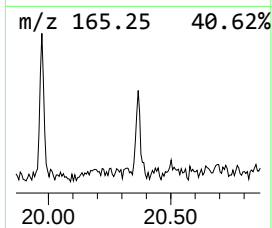
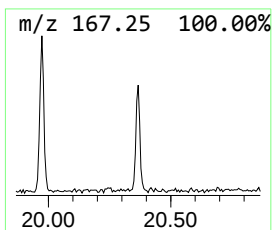
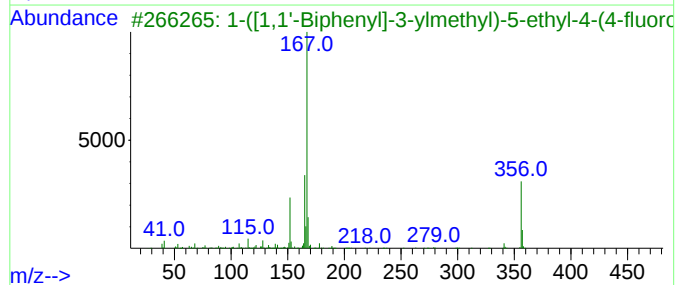
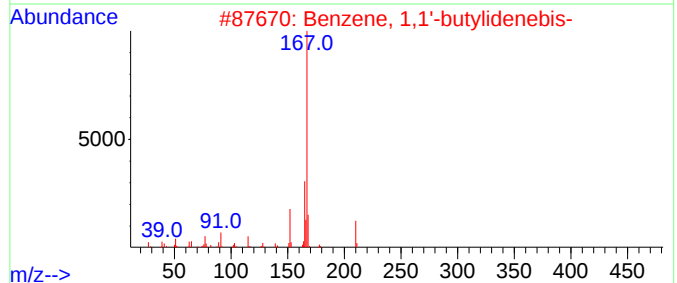
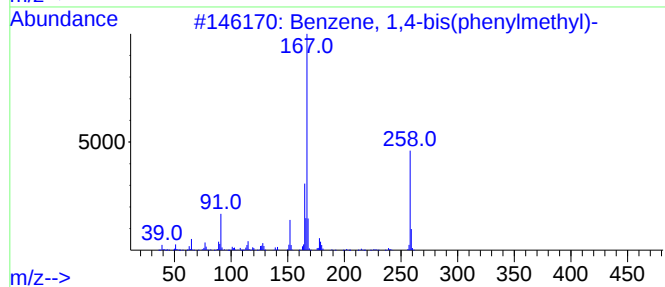
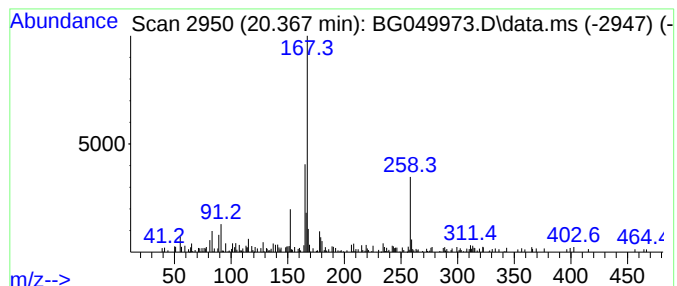
Instrument :
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ClientSampleId :
PT-3-082421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzene, 1,4-bis(phenylmeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.367	3.47 ng	65998	Chrysene-d12	21.671	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-bis(phenylmethyl)-	258	C20H18	000793-23-7	87
2	Benzene, 1,1'-butylidenebis-	210	C16H18	000719-79-9	74
3	1-([1,1'-Biphenyl]-3-ylmethyl)-5...	356	C24H21FN2	1000465-00-1	74
4	2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	74
5	Benzene, 1,1'-(chloromethylene)bis-	202	C13H11Cl	000090-99-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049973.D
Acq On : 25 Aug 2021 18:17
Operator : CG/JU
Sample : M3528-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PT-3-082421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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
Benzene, 1-chlo...	6.944	35.8	ng	376130	1	7.983	210285	20.0
Benzene, 1-chlo...	7.055	19.9	ng	209503	1	7.983	210285	20.0
Ethanol, 2-[2-(...	10.562	4.3	ng	65025	2	10.803	303323	20.0
1,1'-Biphenyl, ...	14.028	5.2	ng	102763	3	14.639	396383	20.0
Naphthalene, 1,...	16.354	2.9	ng	62806	4	17.394	431230	20.0
2-Methylbenzhyd...	16.607	3.6	ng	78169	4	17.394	431230	20.0
unknown16.871	16.871	2.3	ng	48458	4	17.394	431230	20.0
Phosphonous dic...	17.993	8.1	ng	174739	4	17.394	431230	20.0
Benzene, 1,4-bi...	20.367	3.5	ng	65998	5	21.671	380837	20.0