

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121423\
 Data File : BG060021.D
 Acq On : 14 Dec 2023 21:04
 Operator : MA/JU
 Sample : 05718-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-LIQUID-20231206

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060021.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.141	5	9	25	rVB	891474	1717477	18.94%	4.849%
2	5.521	408	414	422	rBV	698850	1162462	12.82%	3.282%
3	7.107	677	684	695	rBV	502777	820193	9.05%	2.316%
4	7.953	822	828	836	rBV	368487	610414	6.73%	1.724%
5	9.117	1018	1026	1037	rBV	1174201	1998446	22.04%	5.643%
6	10.756	1298	1305	1312	rBV	475708	860848	9.49%	2.431%
7	13.218	1716	1724	1733	rBV	3527422	5296485	58.42%	14.955%
8	14.593	1949	1958	1965	rBV	839243	1301974	14.36%	3.676%
9	16.079	2205	2211	2218	rBV	3730775	5586939	61.62%	15.775%
10	17.336	2420	2425	2433	rBV	1164050	1817970	20.05%	5.133%
11	18.235	2574	2578	2581	rBV4	109082	145826	1.61%	0.412%
12	19.963	2866	2872	2878	rBV	7026243	9066355	100.00%	25.599%
13	20.580	2974	2977	2983	rVB2	89061	113197	1.25%	0.320%
14	21.608	3146	3152	3158	rBV2	1134673	1817713	20.05%	5.132%
15	22.395	3282	3286	3296	rBV5	77565	152126	1.68%	0.430%
16	23.277	3431	3436	3447	rVB7	102795	257210	2.84%	0.726%
17	24.334	3608	3616	3624	rVB3	101922	274939	3.03%	0.776%
18	24.798	3684	3695	3703	rBV	678050	1938234	21.38%	5.473%
19	25.621	3827	3835	3850	rVB6	105818	365233	4.03%	1.031%
20	27.225	4102	4108	4109	rBV5	77858	112718	1.24%	0.318%

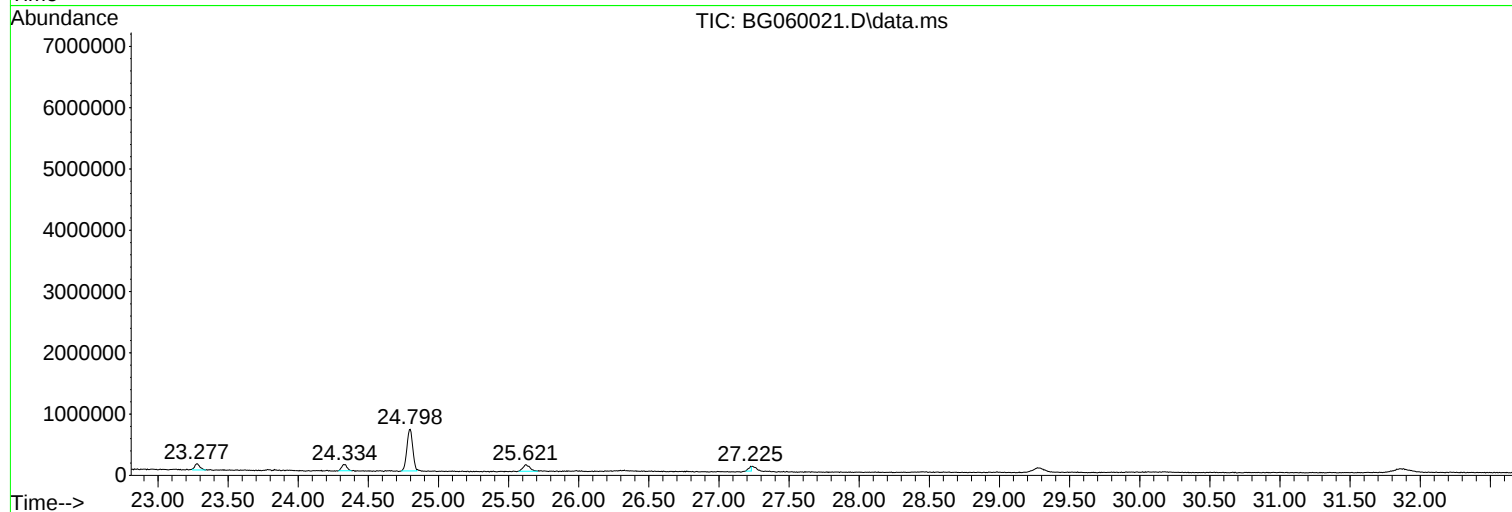
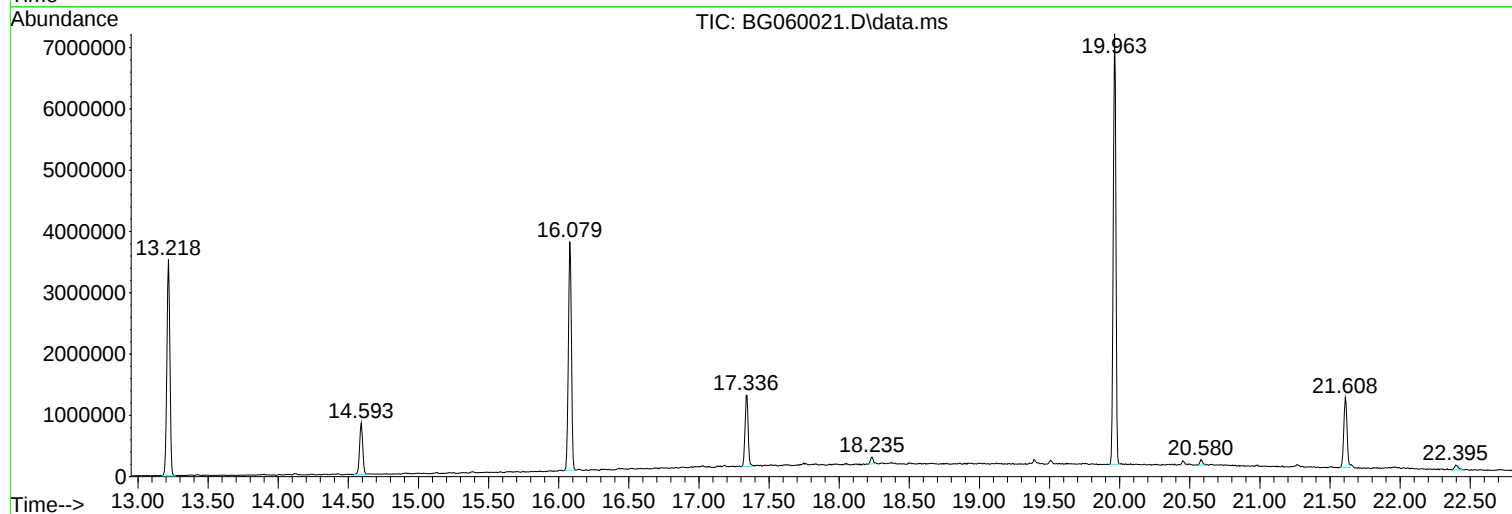
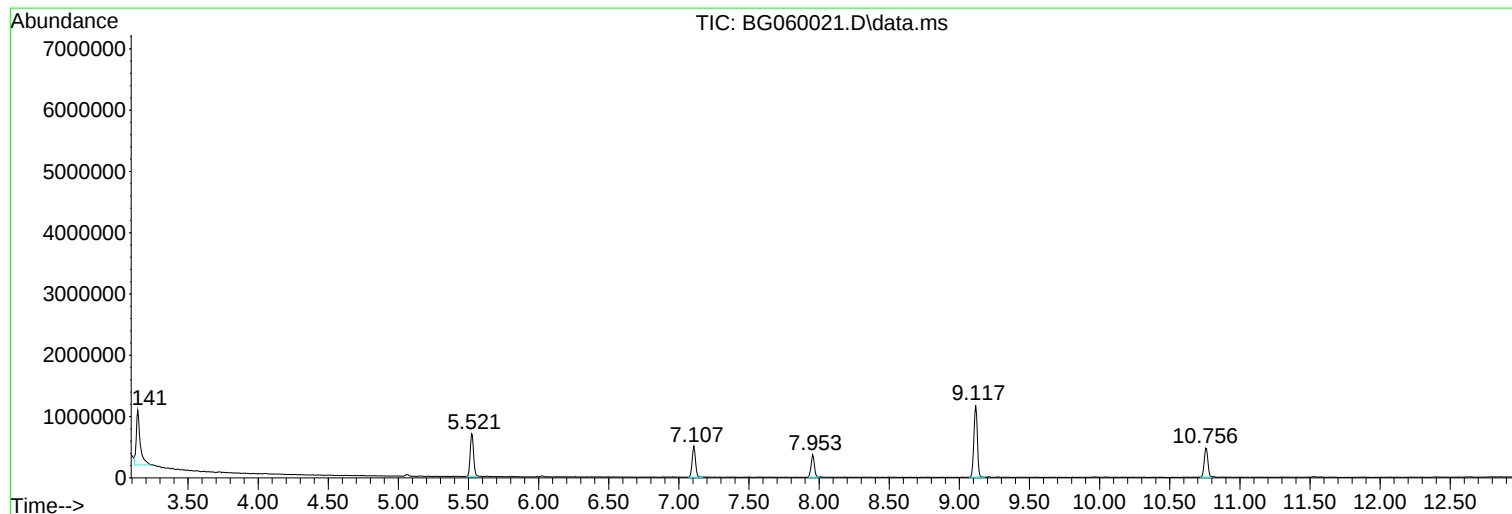
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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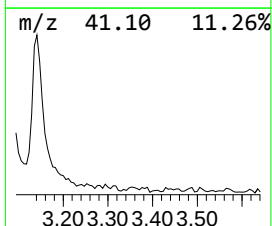
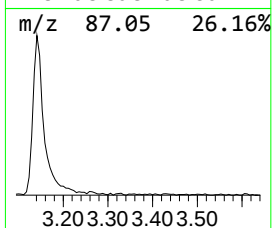
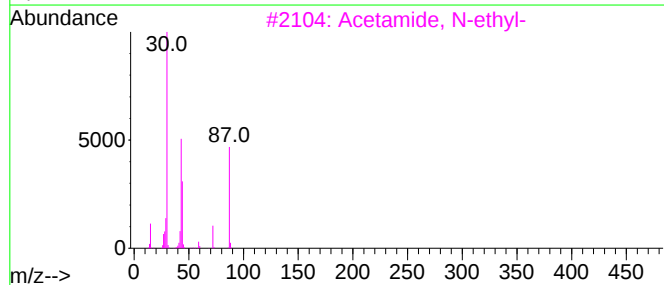
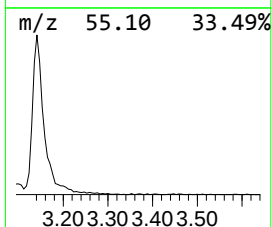
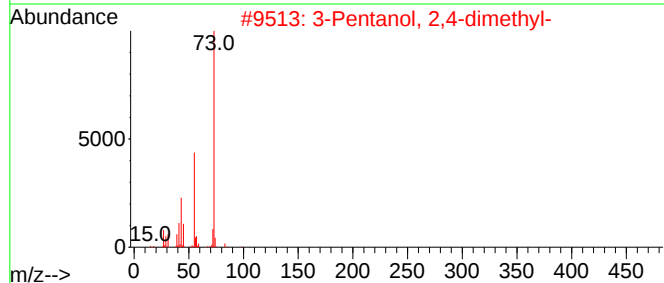
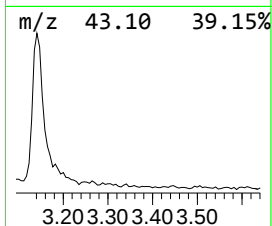
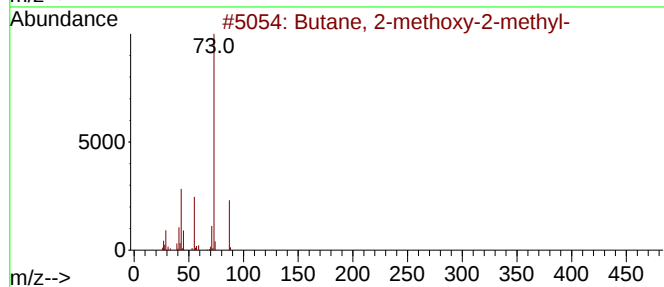
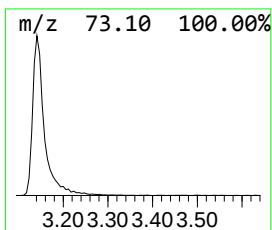
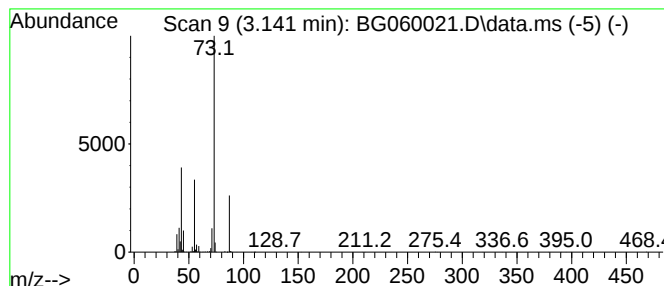
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.141	56.27 ng	1717480	1,4-Dichlorobenzene-d4	7.953

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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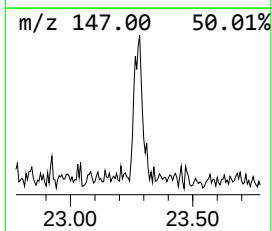
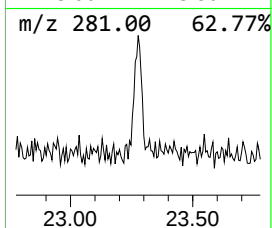
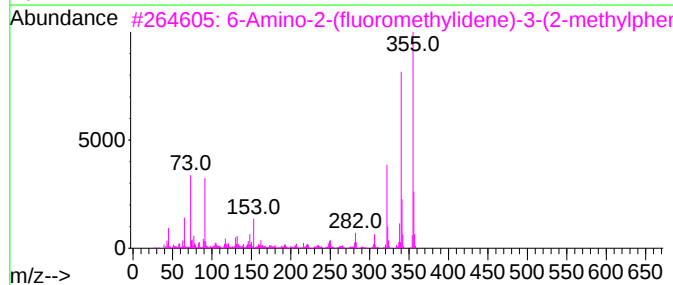
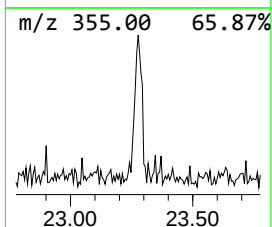
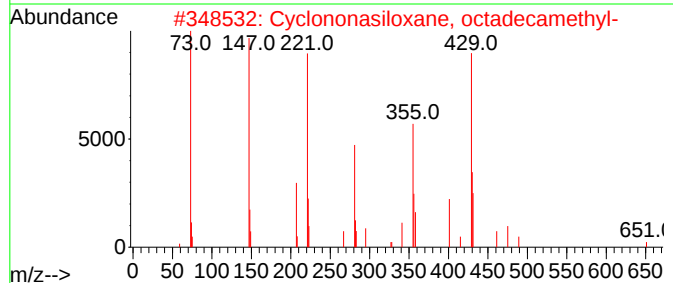
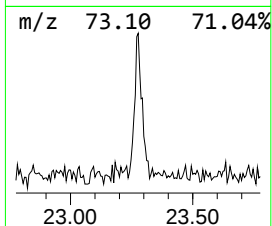
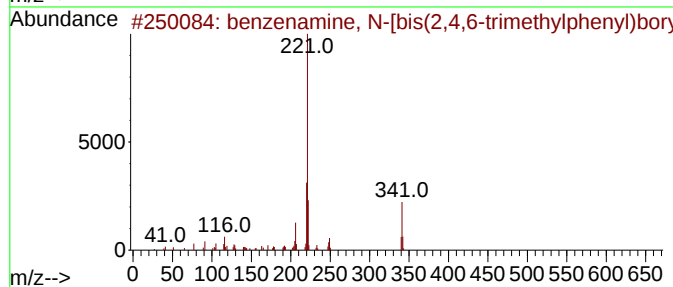
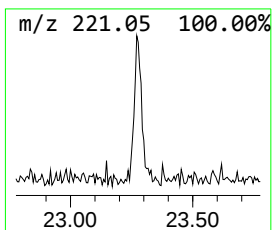
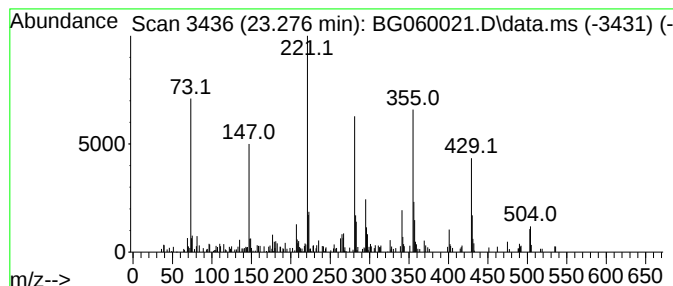
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown23.276 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.276	2.65 ng	257210	Perylene-d12	24.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	22
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	14
3			6-Amino-2-(fluoromethylidene)-3-...	355	C19H22FN3OSi	1010408-41-2	14
4			3-(4-N,N-Dimethylaminophenyl)pro...	355	C17H26N05P	066564-08-7	11
5			Oxazepam, 2TMS derivative	430	C21H27ClN2O2Si2	055319-93-2	11



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WC-LIQUID-20231206

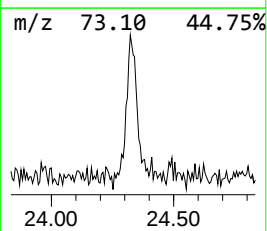
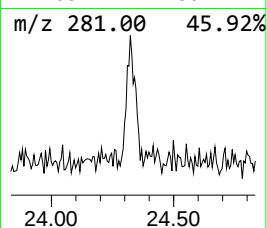
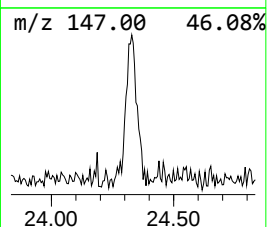
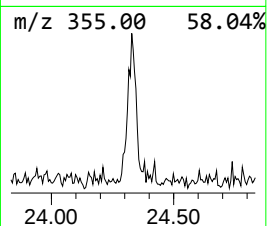
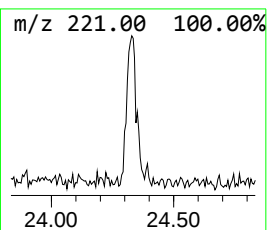
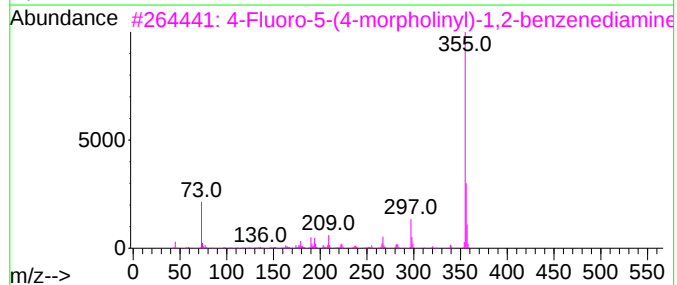
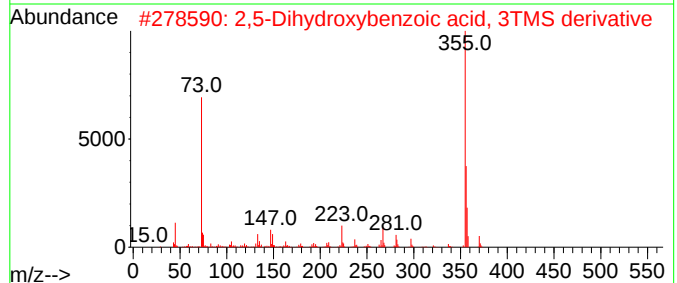
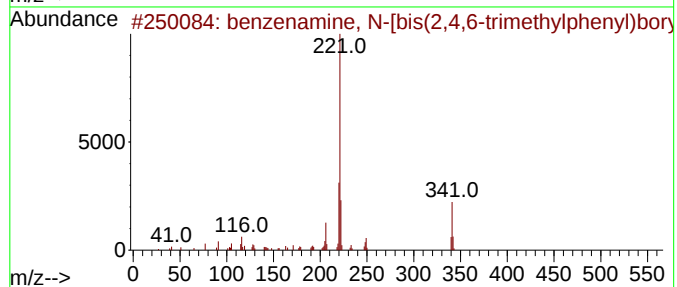
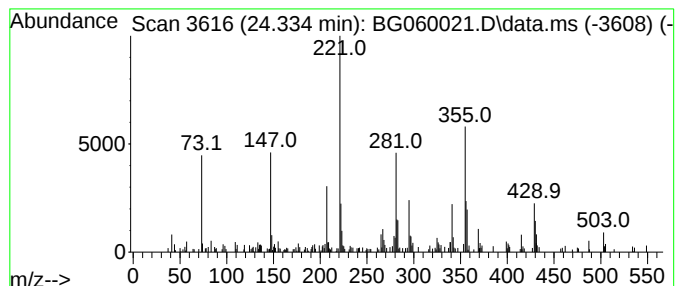
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown24.334 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.334	2.84 ng	274939	Perylene-d12	24.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	35
2			2,5-Dihydroxybenzoic acid, 3TMS ...	370	C16H30O4Si3	003618-20-0	25
3			4-Fluoro-5-(4-morpholinyl)-1,2-b...	355	C16H30FN3OSi2	1000479-80-2	25
4			1,2-Dibenzoyl-3-phenylcyclopropane	326	C23H18O2	029128-64-1	20
5			Methylergonovine	339	C20H25N3O2	000113-42-8	20



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Misc :
ALS Vial : 10 Sample Multiplier: 1

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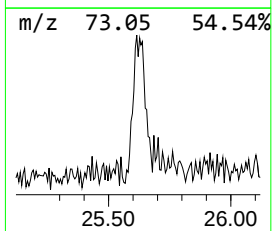
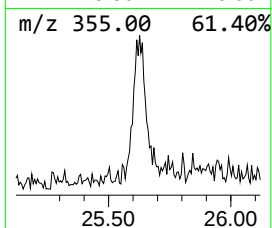
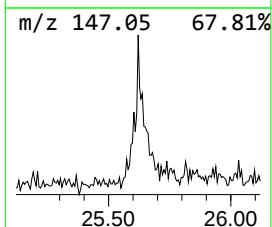
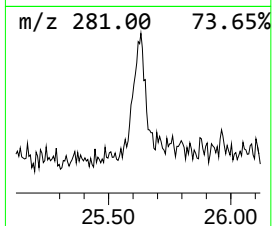
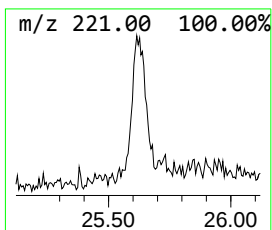
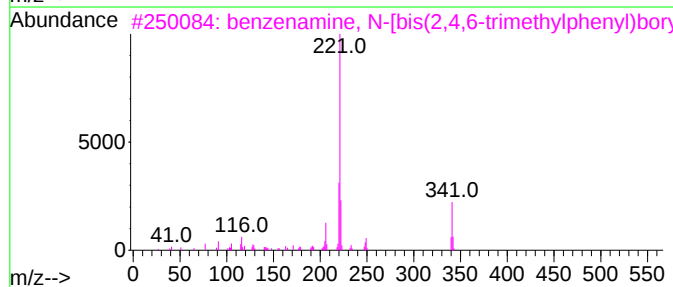
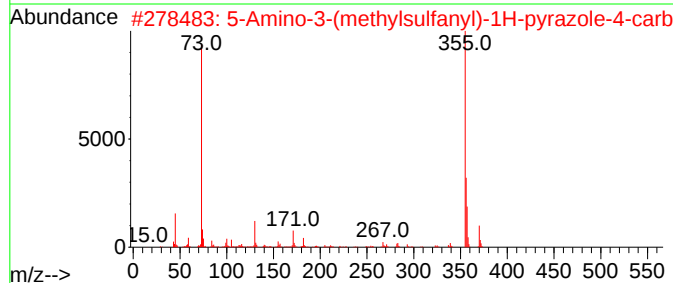
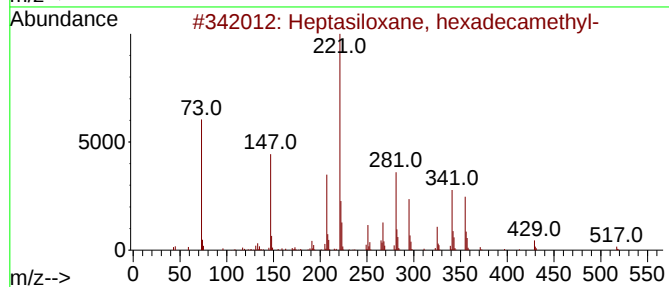
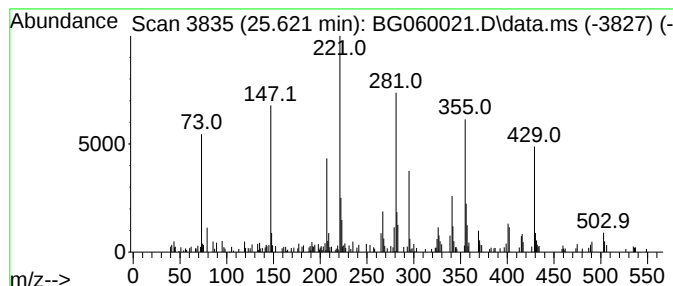
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown25.621 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.621	3.77 ng	365233	Perylene-d12	24.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	35
2			5-Amino-3-(methylsulfanyl)-1H-py...	370	C14H30N4SSi3	1000474-62-1	25
3			benzenamine, N-[bis(2,4,6-trimet...	341	C24H28BN	1000398-20-2	18
4			3-Phenyl oxindole, BSTFA derivative	281	C17H19NOSi	1000458-51-5	11
5			1-heptyl-3-(naphthalen-1-ylmethy...	355	C26H29N	1000372-24-5	11



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.141	56.3	ng	1717480	1	7.953	610414	20.0
unknown23.276	23.276	2.6	ng	257210	6	24.798	1938230	20.0
unknown24.334	24.334	2.8	ng	274939	6	24.798	1938230	20.0
unknown25.621	25.621	3.8	ng	365233	6	24.798	1938230	20.0