

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
 Data File : BG055847.D
 Acq On : 30 Nov 2022 18:30
 Operator : CG/JU
 Sample : N5809-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HOWE-DRUM-C-1129

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055847.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.659	228	233	239	rBV	28959	49933	3.33%	0.669%
2	5.276	330	338	349	rVB	422976	683376	45.62%	9.162%
3	5.764	413	421	434	rBV	611971	1087870	72.62%	14.584%
4	6.375	519	525	533	rVB	37516	60390	4.03%	0.810%
5	7.380	687	696	711	rBV	611578	1137371	75.93%	15.248%
6	7.509	711	718	725	rBV	42281	82167	5.49%	1.102%
7	8.226	832	840	847	rBV	154778	269568	18.00%	3.614%
8	9.395	1030	1039	1051	rBV	307709	566742	37.83%	7.598%
9	11.052	1313	1321	1329	rBV	203544	370388	24.73%	4.966%
10	13.472	1726	1733	1741	rVB	1012394	1497937	100.00%	20.082%
11	14.847	1962	1967	1973	rVB	303204	466823	31.16%	6.258%
12	16.334	2214	2220	2228	rBV	672841	1186565	79.21%	15.908%

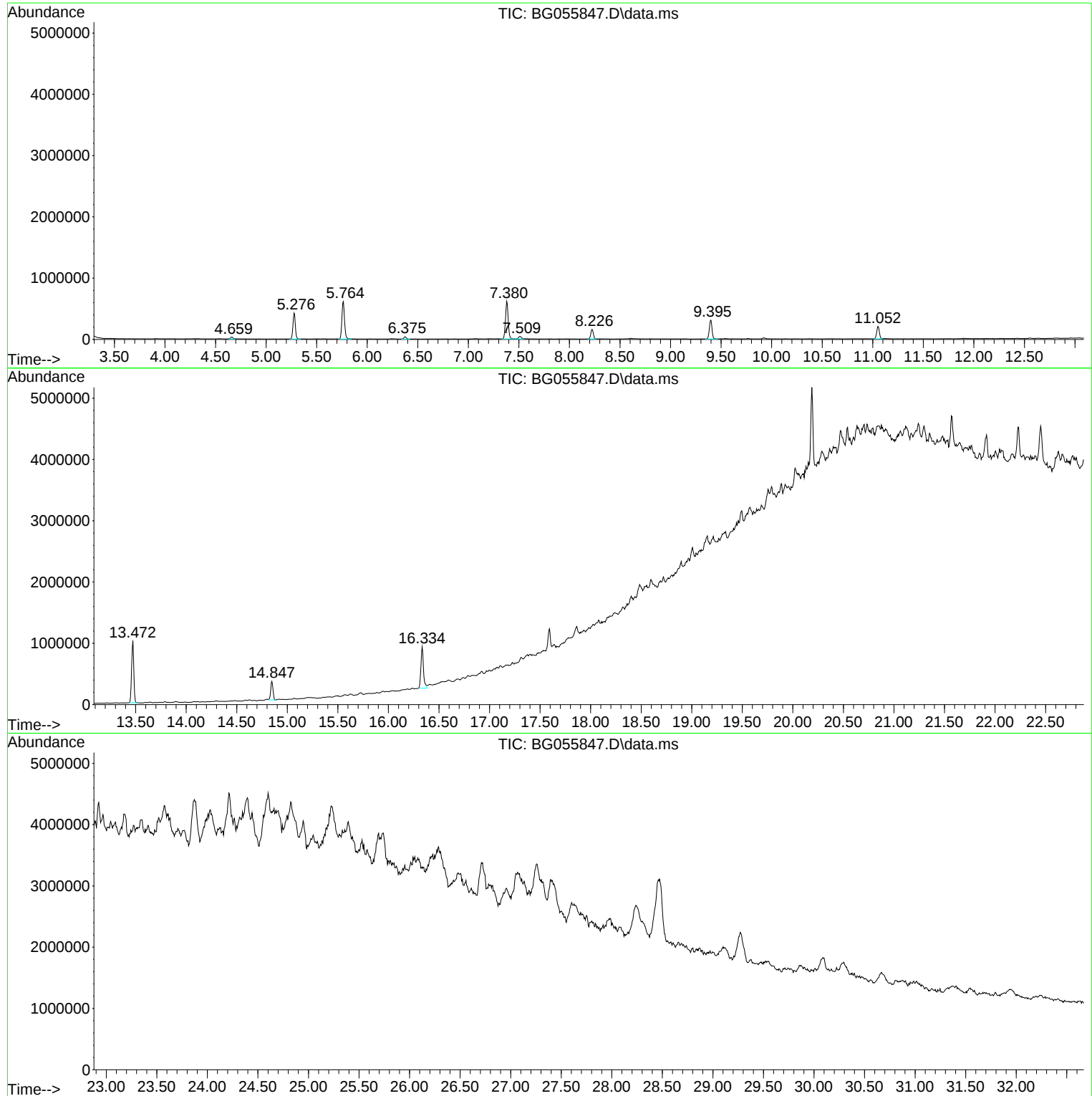
Sum of corrected areas: 7459130

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
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TIC Library : C:\Database\NIST20.L
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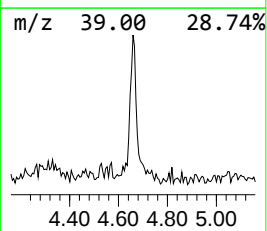
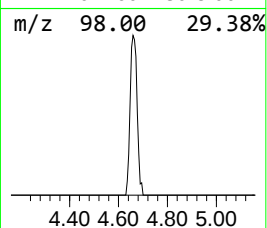
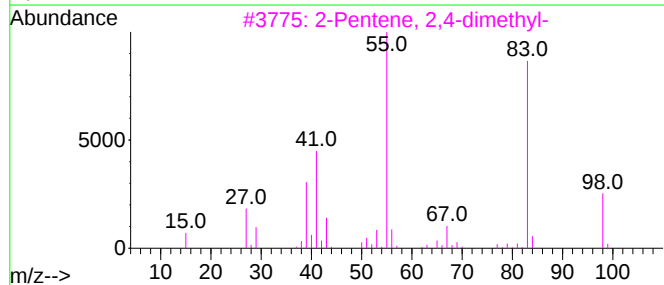
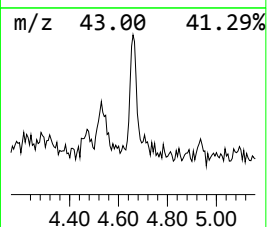
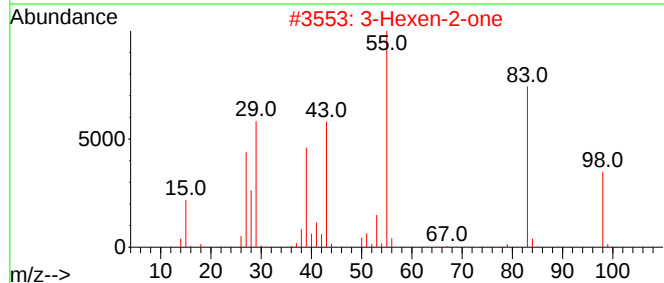
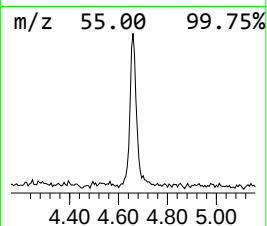
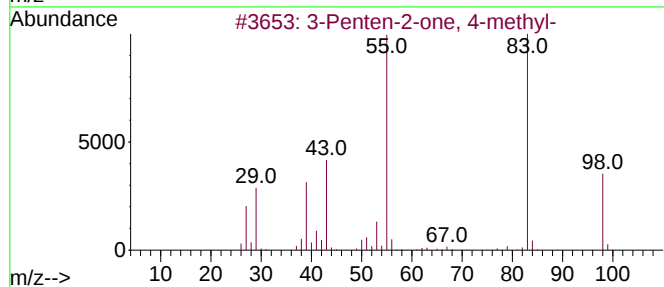
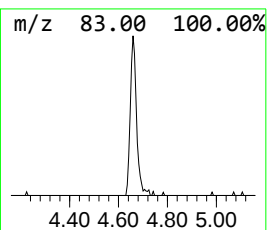
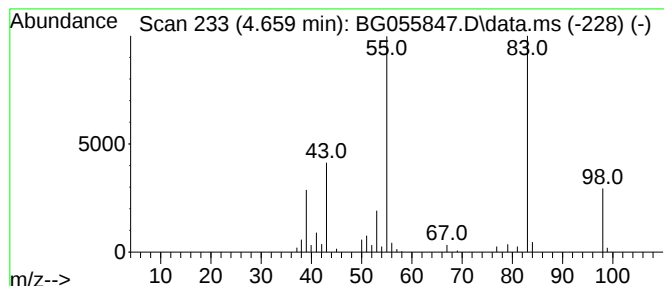
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.659	3.70 ng	49933	1,4-Dichlorobenzene-d4	8.226

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	87
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	64



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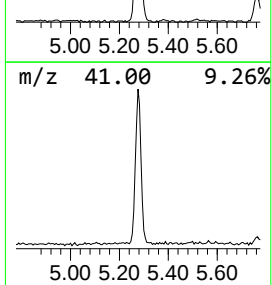
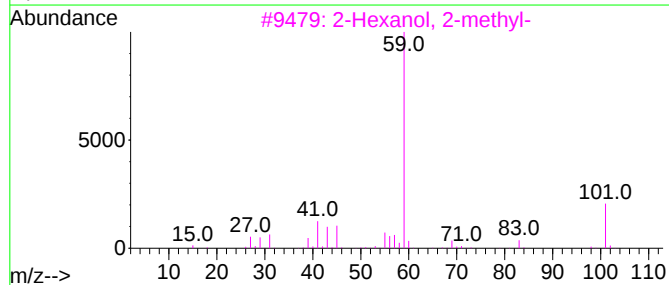
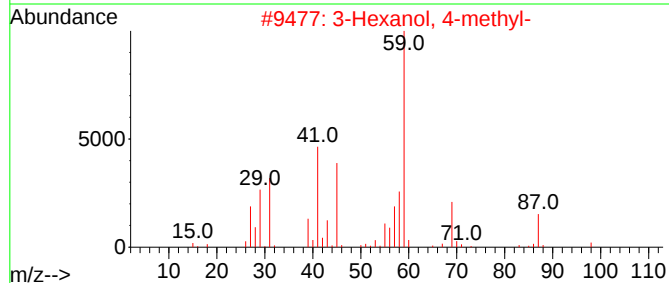
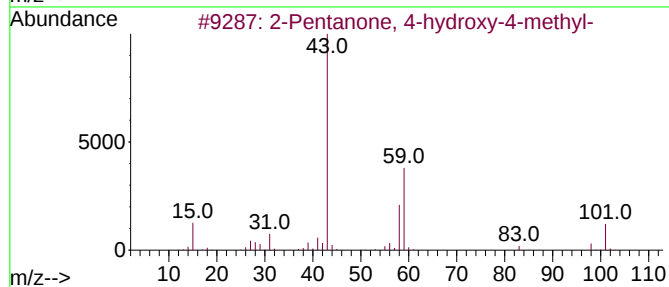
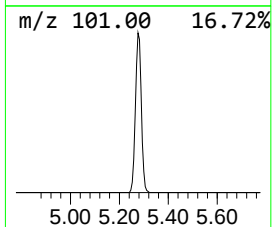
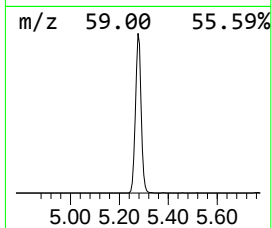
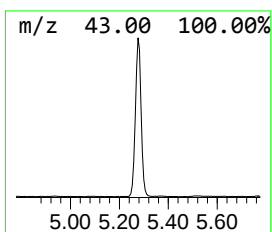
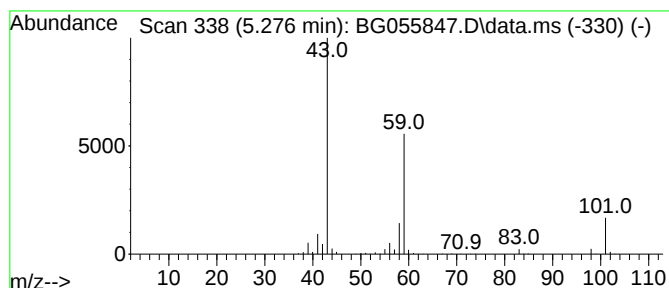
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.276	50.70 ng	683376	1,4-Dichlorobenzene-d4	8.226

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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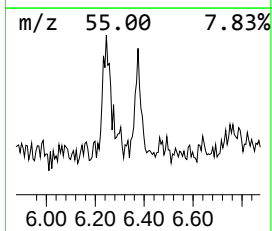
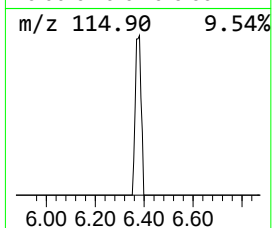
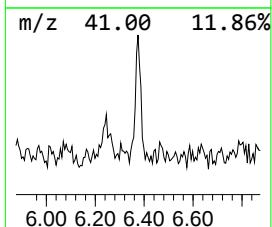
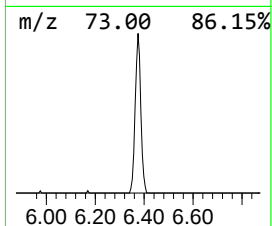
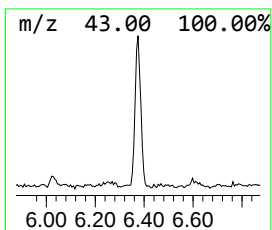
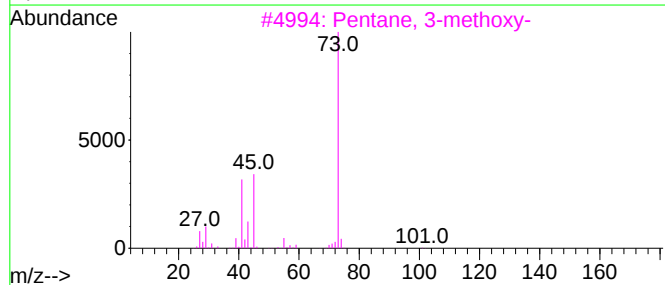
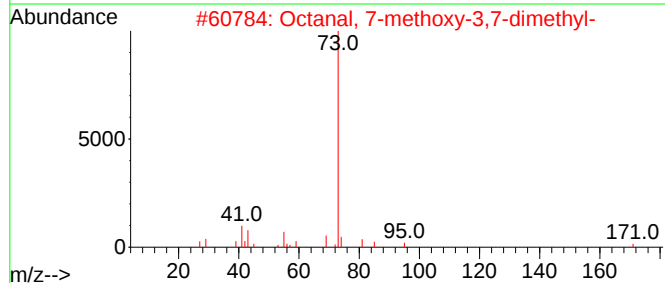
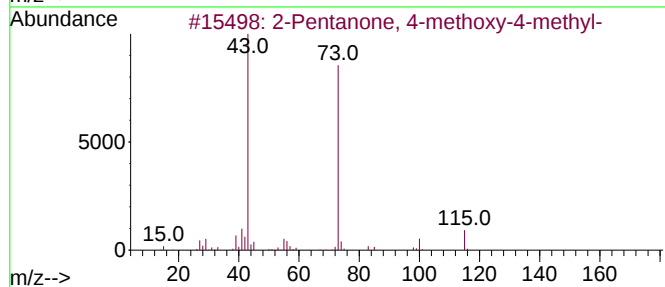
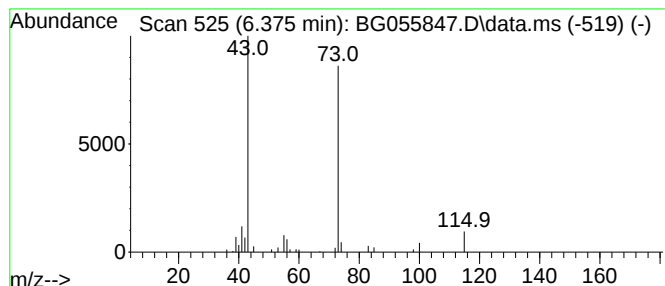
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.375	4.48 ng	60390	1,4-Dichlorobenzene-d4	8.226

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9



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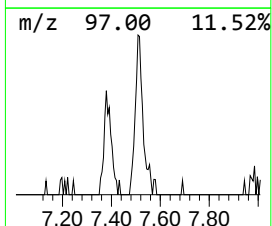
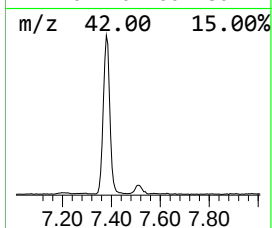
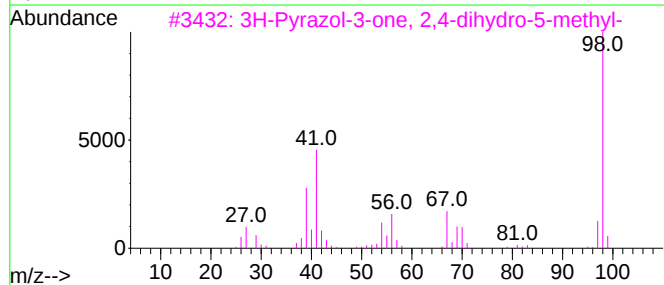
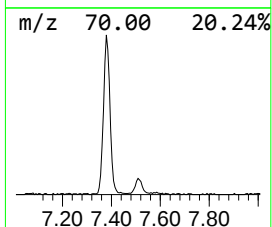
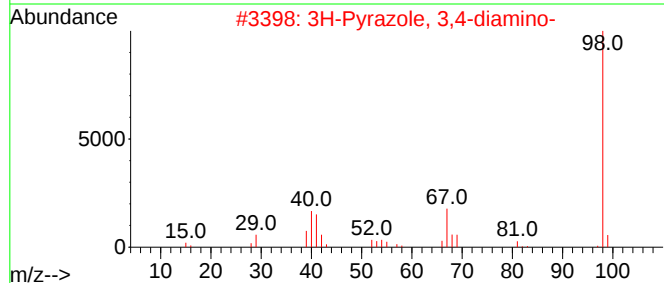
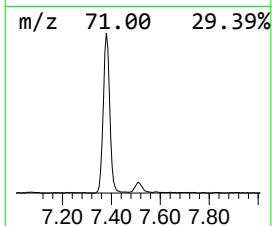
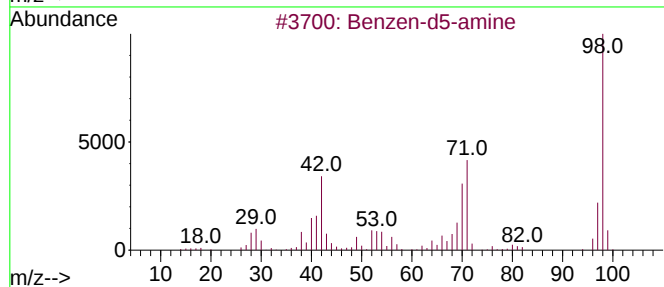
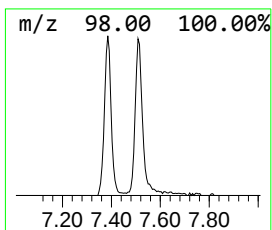
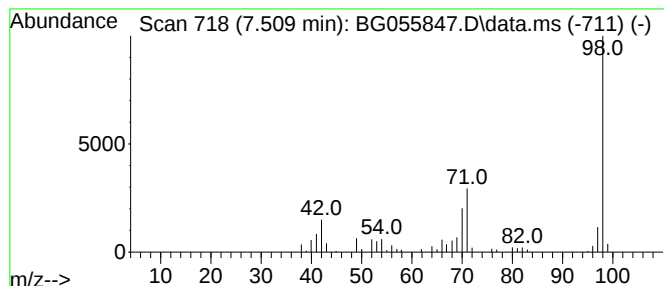
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Peak Number 4 Benzen-d5-amine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.509	6.10 ng	82167	1,4-Dichlorobenzene-d4	8.226

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzen-d5-amine	98	C6H2D5N	004165-61-1	80
2			3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	43
3			3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	40
4			1,3,4-Thiadiazole-2(3H)-thione, ...	229	C9H15N3S2	1000338-18-2	38
5			1H-Tetrazaborole, 4,5-dihydro-1,...	98	C2H7BN4	006982-51-0	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.659	3.7	ng	49933	1	8.226	269568	20.0
2-Pentanone, 4-...	5.276	50.7	ng	683376	1	8.226	269568	20.0
2-Pentanone, 4-...	6.375	4.5	ng	60390	1	8.226	269568	20.0
Benzen-d5-amine	7.509	6.1	ng	82167	1	8.226	269568	20.0