

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
 Data File : BF124803.D
 Acq On : 27 Jul 2021 20:25
 Operator : JU/CG
 Sample : M3159-13
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210545-COM-18

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_F\METHODS\8270-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124803.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	9	13	17	rBB	5435	6607	2.41%	0.499%
2	5.487	574	578	581	rBV	149242	154348	56.33%	11.654%
3	6.498	745	750	753	rBB	160203	159865	58.34%	12.071%
4	6.869	810	813	816	rBB	42308	30857	11.26%	2.330%
5	7.434	904	909	912	rBB	120931	105491	38.50%	7.965%
6	8.051	1012	1014	1017	rBB	5925	4574	1.67%	0.345%
7	8.151	1028	1031	1034	rBB	58001	41539	15.16%	3.136%
8	9.228	1210	1214	1217	rBV	240722	208383	76.05%	15.734%
9	9.910	1326	1330	1333	rBB	60899	50156	18.30%	3.787%
10	10.698	1460	1464	1467	rBV	174142	145401	53.06%	10.979%
11	11.398	1579	1583	1586	rBB	67761	59318	21.65%	4.479%
12	12.986	1848	1853	1856	rBV	309452	274022	100.00%	20.690%
13	13.880	2003	2005	2012	rBB2	3222	4596	1.68%	0.347%
14	14.033	2027	2031	2034	rBB	54415	43878	16.01%	3.313%
15	14.880	2172	2175	2178	rBB	4707	3687	1.35%	0.278%
16	15.510	2277	2282	2287	rBB	27665	31674	11.56%	2.392%

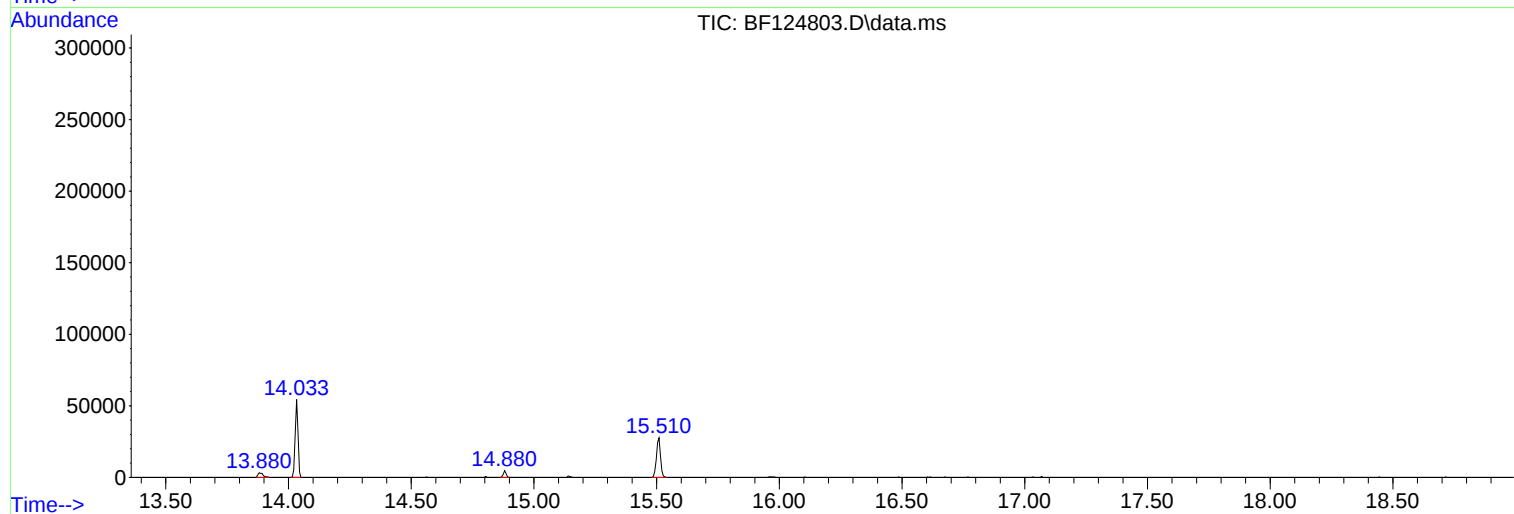
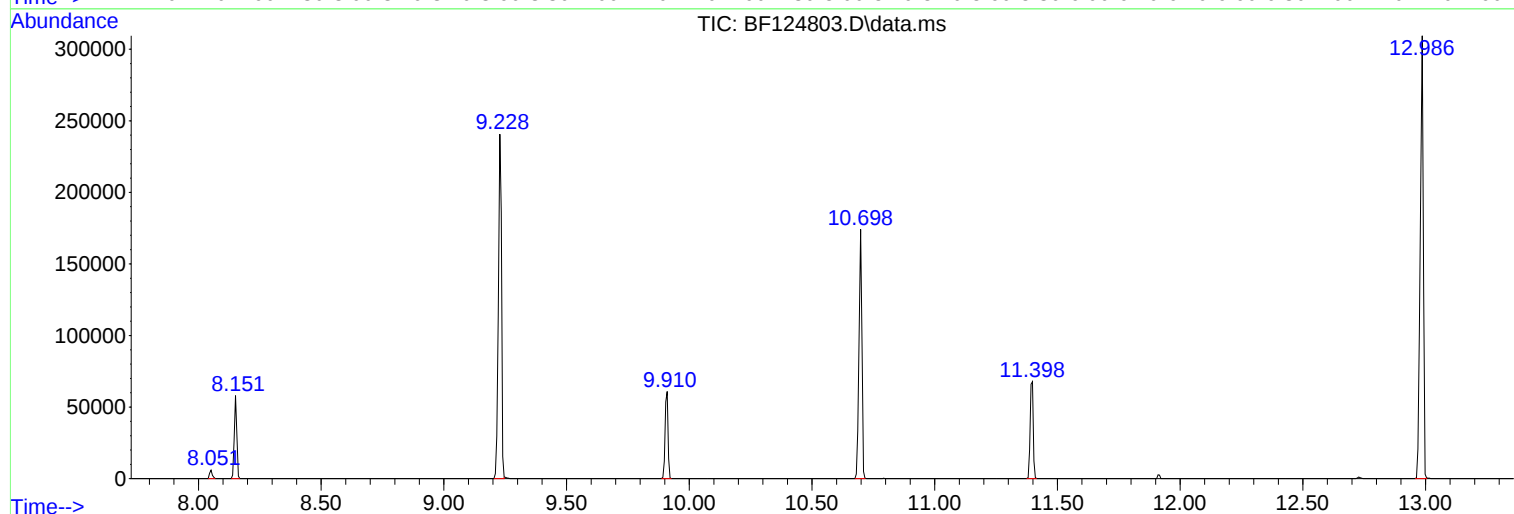
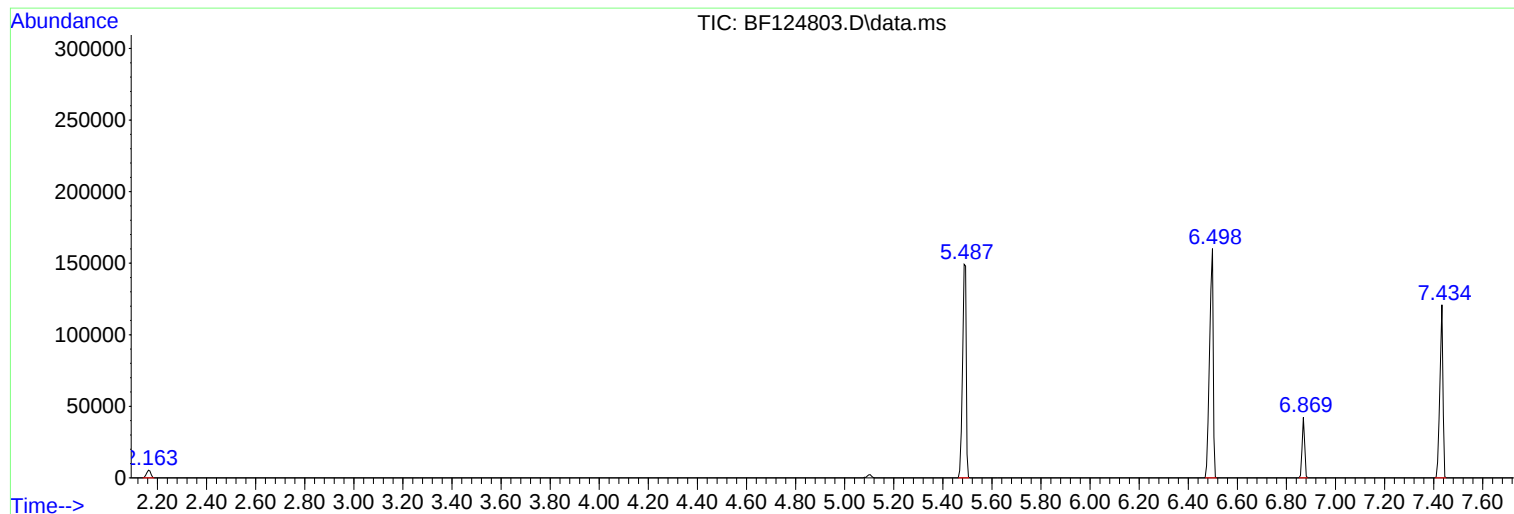
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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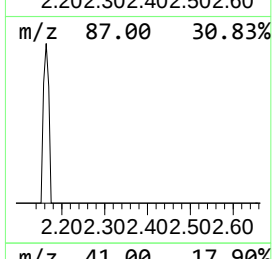
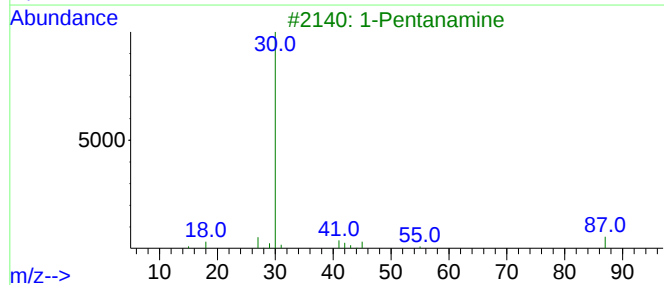
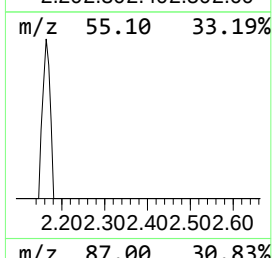
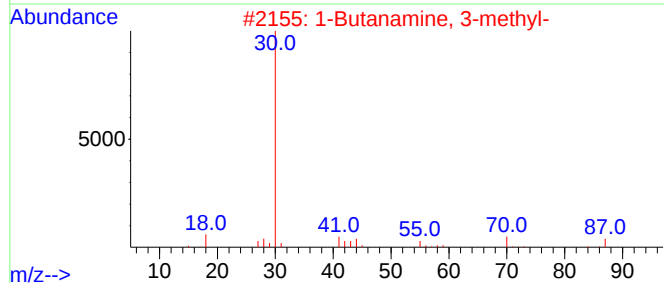
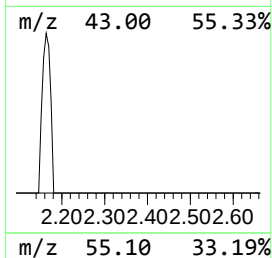
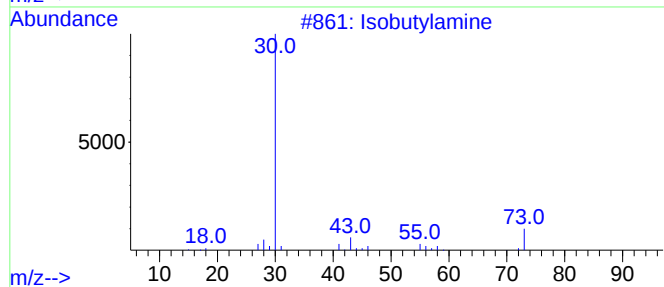
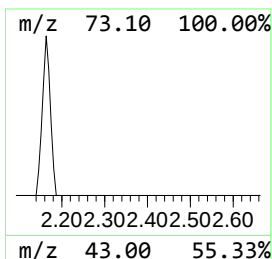
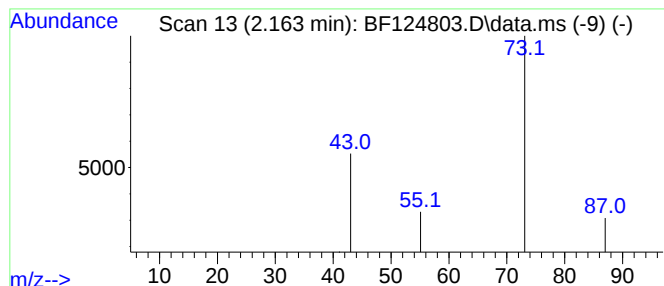
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 unknown2.163 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	4.28 ng	6607	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutylamine	73	C4H11N	000078-81-9	4
2			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
3			1-Pentanamine	87	C5H13N	000110-58-7	3
4			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	2
5			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	2



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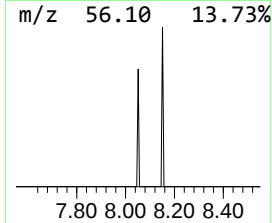
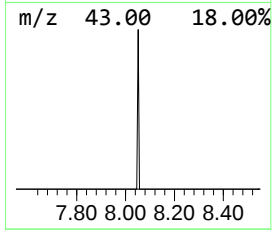
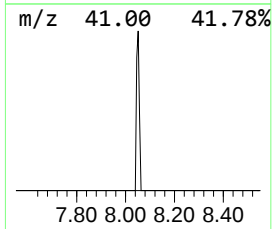
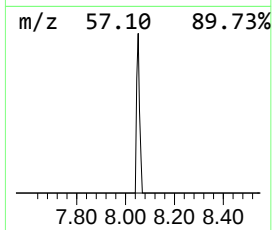
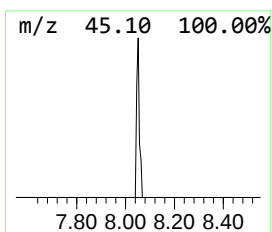
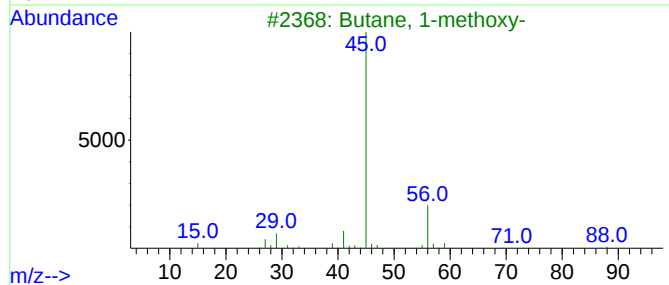
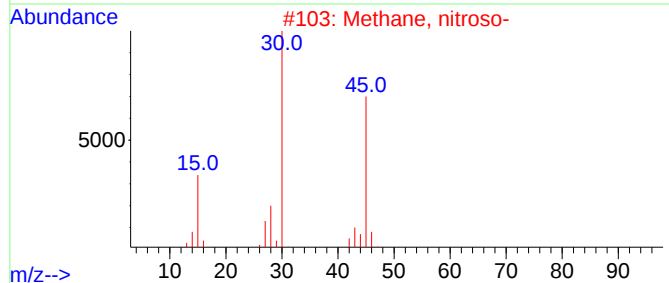
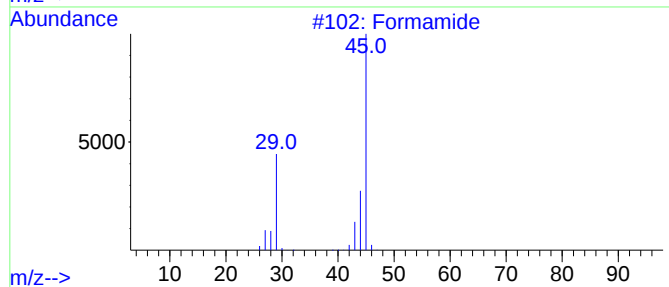
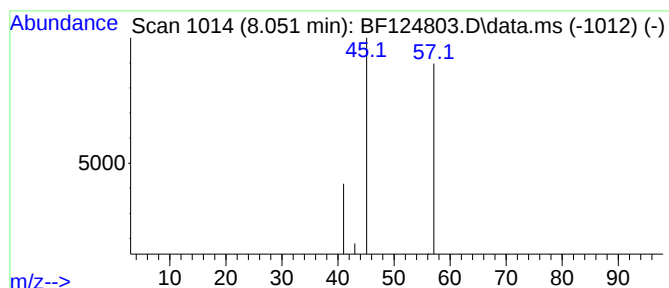
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Peak Number 2 unknown8.051 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	2.20 ng	4574	Naphthalene-d8	8.151

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Formamide	45	CH3NO	000075-12-7	3
2		Methane, nitroso-	45	CH3NO	000865-40-7	3
3		Butane, 1-methoxy-	88	C5H12O	000628-28-4	1
4		Ethylamine	45	C2H7N	000075-04-7	1
5		3-Hydroxy-2-methylbutanenitrile	99	C5H9NO	038046-46-7	1



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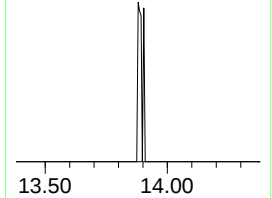
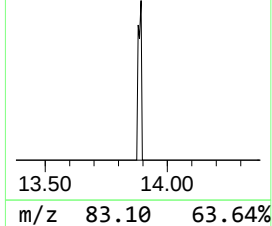
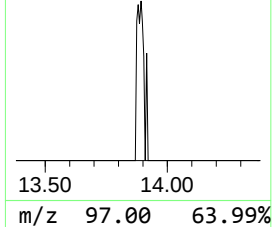
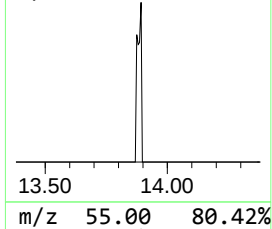
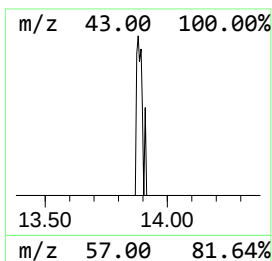
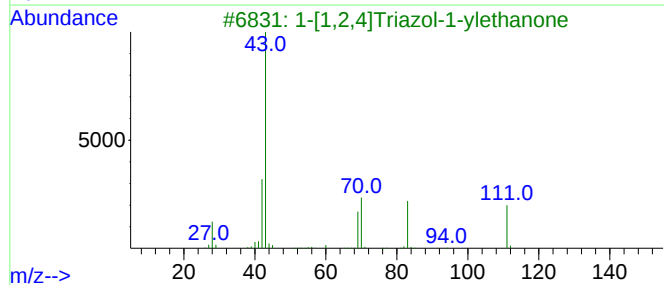
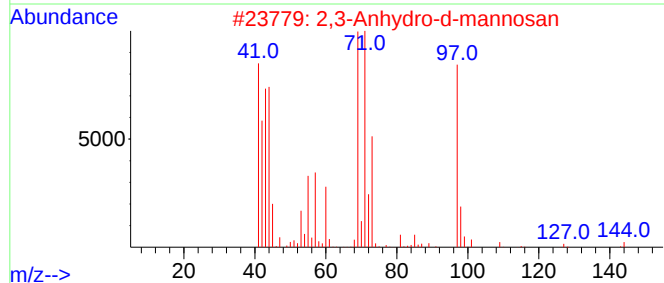
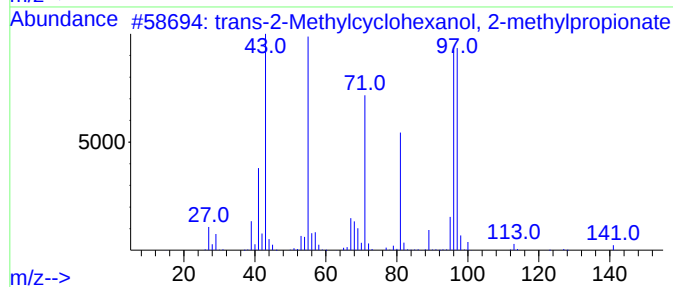
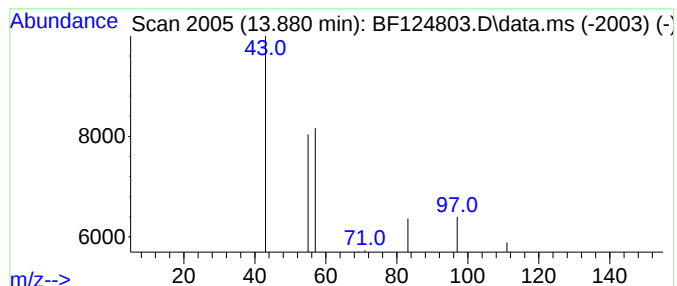
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Peak Number 3 unknown13.880 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.09 ng	4596	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Methylcyclohexanol, 2-me...	184	C11H20O2	1000447-34-0	9
2			2,3-Anhydro-d-mannosan	144	C6H8O4	1000129-98-0	9
3			1-[1,2,4]Triazol-1-ylethanone	111	C4H5N3O	015625-88-4	7
4			1H-1,2,4-Triazole, 3-propyl-	111	C5H9N3	019932-60-6	5
5			Difluoroisocyanatophosphine	111	CF2NOP	1000306-12-1	5



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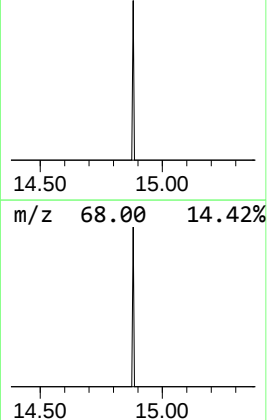
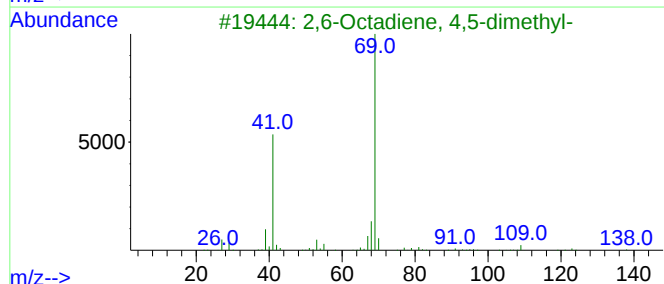
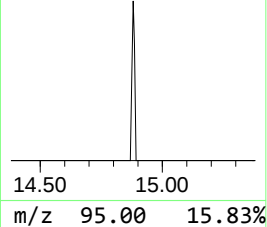
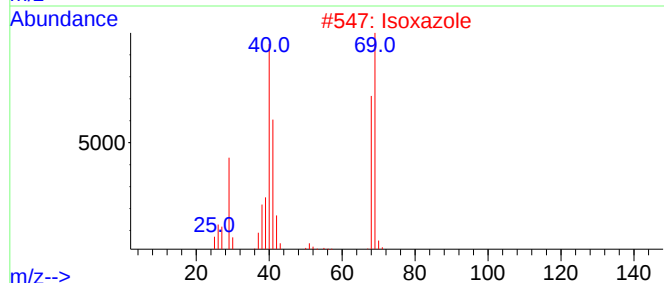
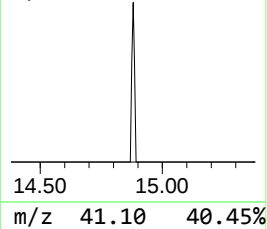
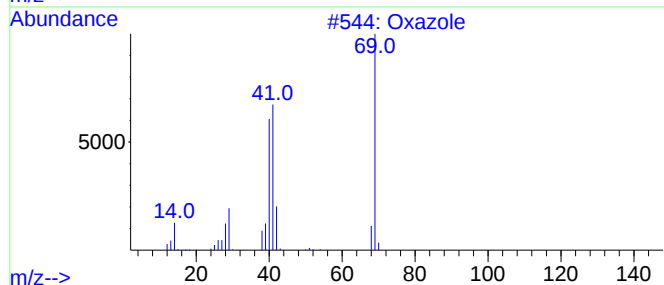
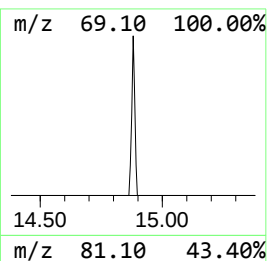
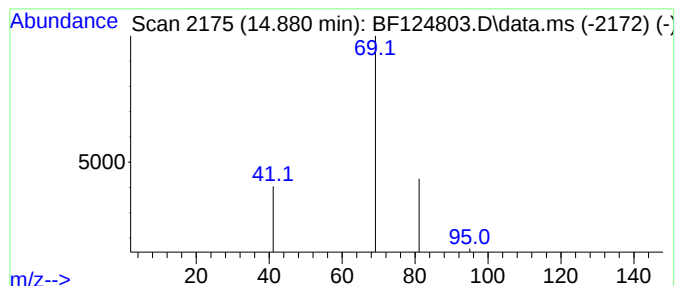
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Peak Number 4 unknown14.880 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.33 ng	3687	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole			69	C3H3NO	000288-42-6	4
2	Isoxazole			69	C3H3NO	000288-14-2	4
3	2,6-Octadiene, 4,5-dimethyl-			138	C10H18	018476-57-8	2
4	Cyclopentane, bromo-			148	C5H9Br	000137-43-9	2
5	1H-1,2,3-Triazole			69	C2H3N3	000288-36-8	2



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown8.051	8.051	2.2	ng	4574	2	8.151	41539	20.0
unknown13.880	13.880	2.1	ng	4596	5	14.033	43878	20.0
unknown14.880	14.880	2.3	ng	3687	6	15.510	31674	20.0