

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072221\
 Data File : BF124698.D
 Acq On : 22 Jul 2021 19:59
 Operator : JU/CG
 Sample : M3093-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210543-COM-16

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: BF124698.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	15	rBB	12867	15227	8.93%	1.442%
2	5.093	508	511	514	rBB	2206	2218	1.30%	0.210%
3	5.481	573	577	580	rBB	145632	136019	79.74%	12.885%
4	6.493	743	749	751	rBB	130697	138689	81.31%	13.138%
5	6.869	810	813	816	rBB	43323	29981	17.58%	2.840%
6	7.428	904	908	911	rBB	94097	91335	53.54%	8.652%
7	8.051	1011	1014	1016	rBB	12223	9673	5.67%	0.916%
8	8.151	1027	1031	1034	rBB	55775	41744	24.47%	3.954%
9	9.228	1210	1214	1217	rBB	225268	170578	100.00%	16.158%
10	9.904	1326	1329	1332	rBB	56217	47866	28.06%	4.534%
11	10.692	1460	1463	1466	rBB	123000	101713	59.63%	9.635%
12	11.392	1579	1582	1585	rBB	62493	46119	27.04%	4.369%
13	11.916	1668	1671	1673	rBB	9215	6943	4.07%	0.658%
14	12.980	1848	1852	1855	rBB	194478	156055	91.49%	14.783%
15	14.027	2027	2030	2033	rBB	37736	30479	17.87%	2.887%
16	14.880	2173	2175	2178	rBB	3413	3004	1.76%	0.285%
17	15.498	2276	2280	2284	rBB	26582	28018	16.43%	2.654%

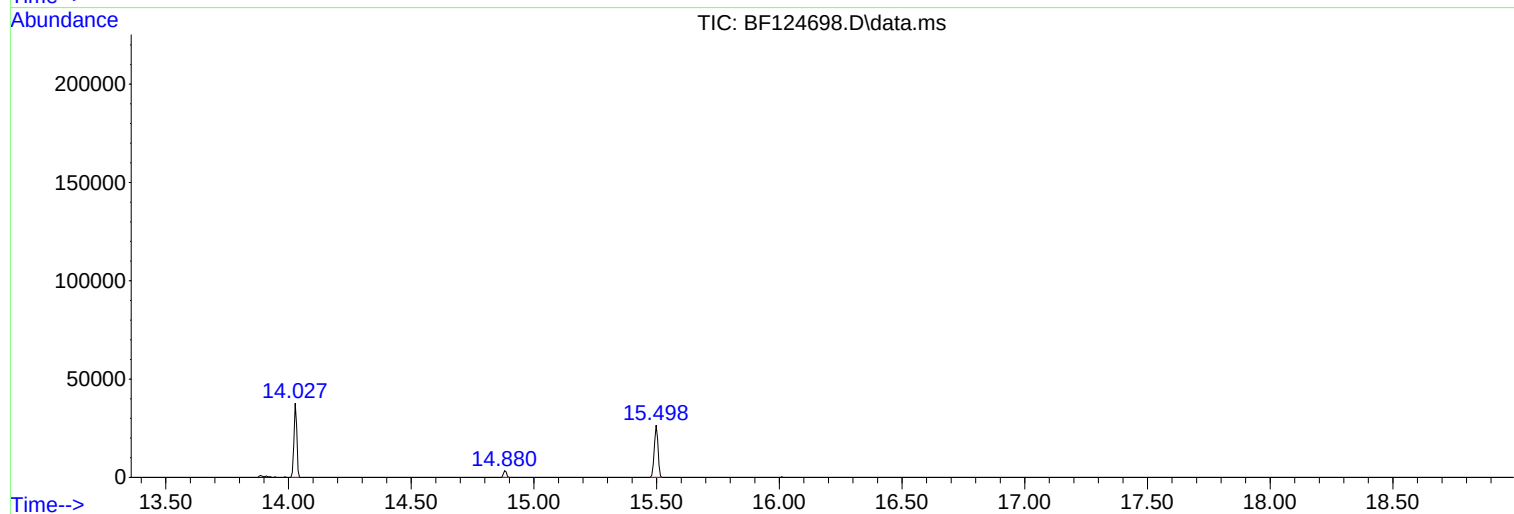
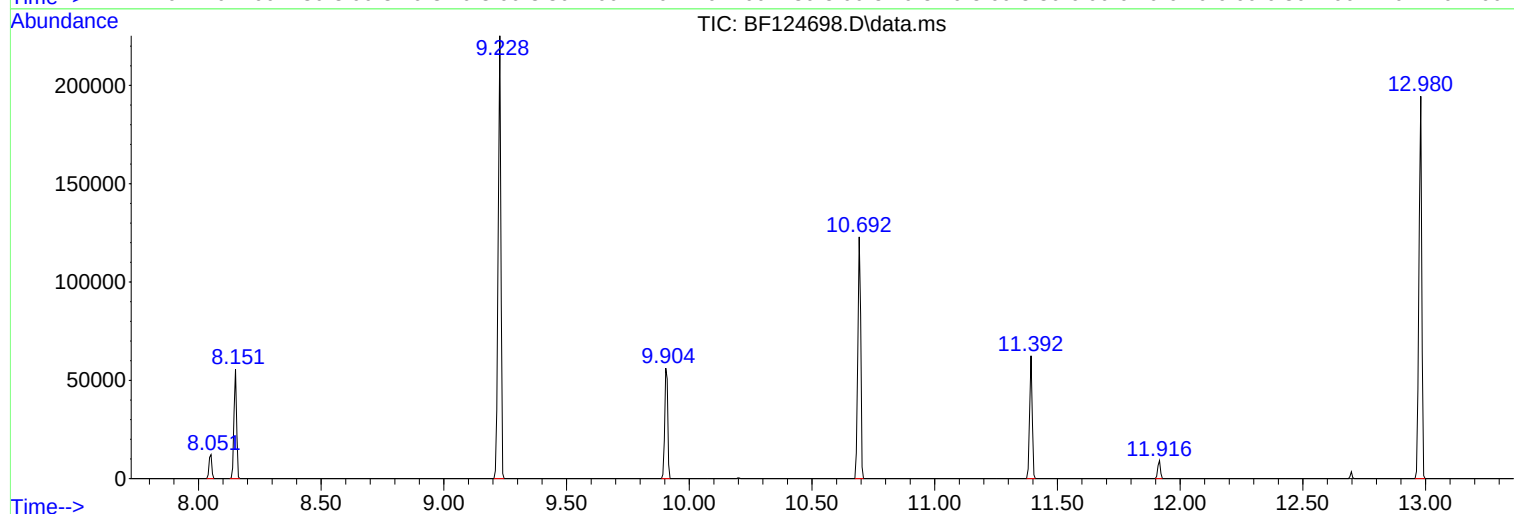
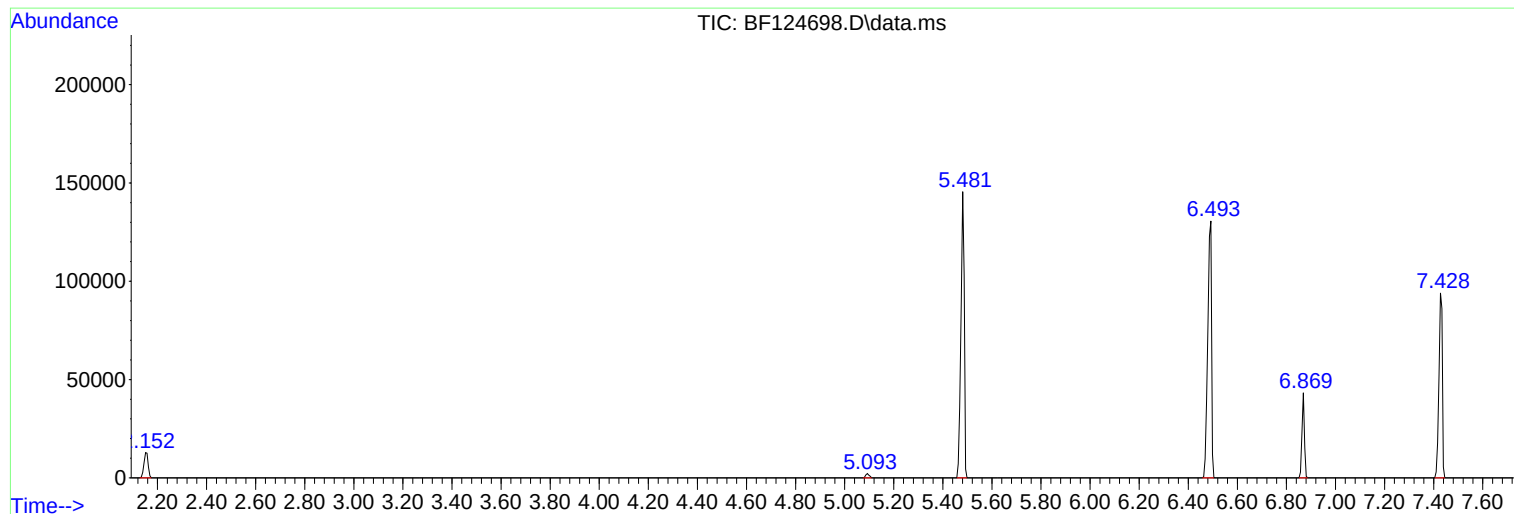
Sum of corrected areas: 1055661

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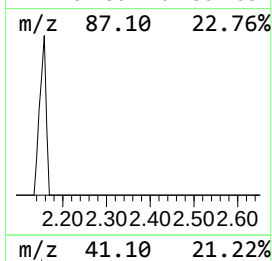
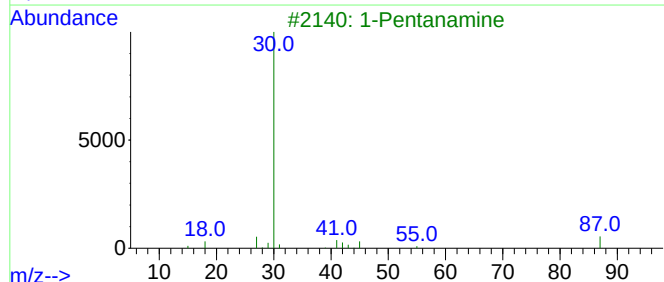
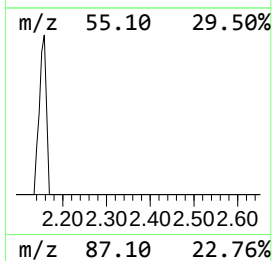
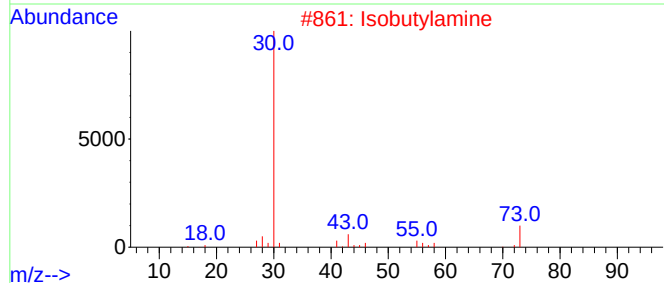
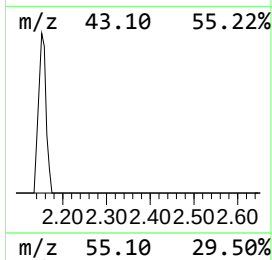
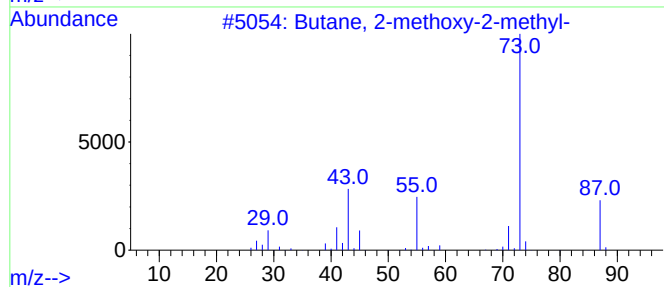
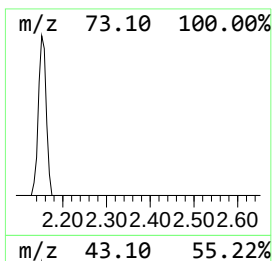
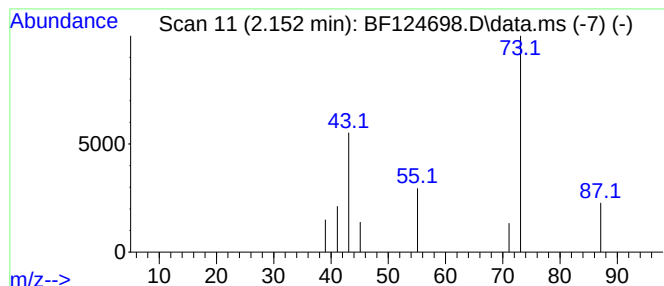
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	10.16 ng	15227	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			Isobutylamine	73	C4H11N	000078-81-9	7
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	4



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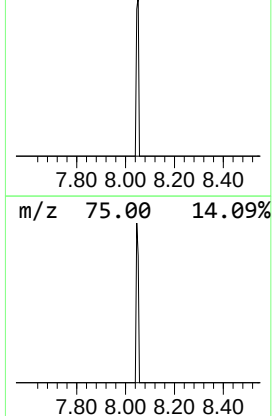
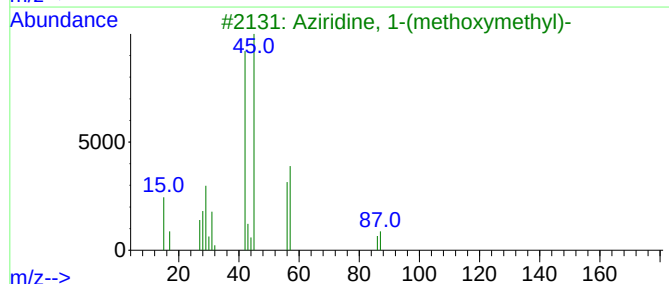
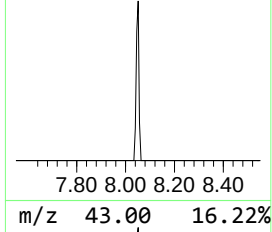
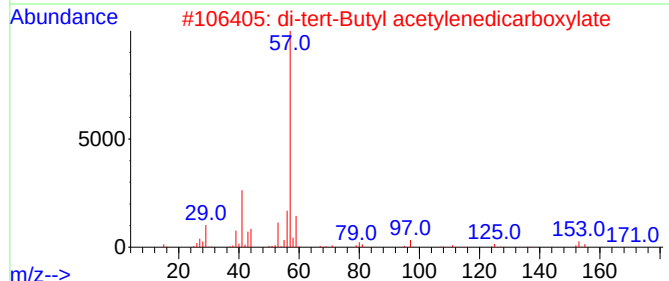
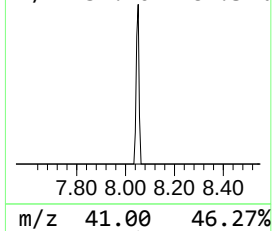
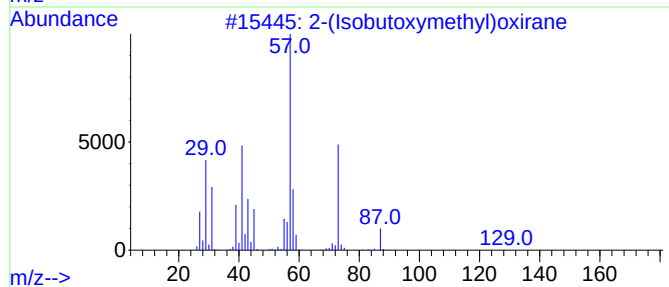
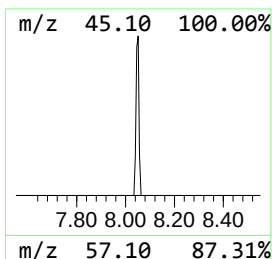
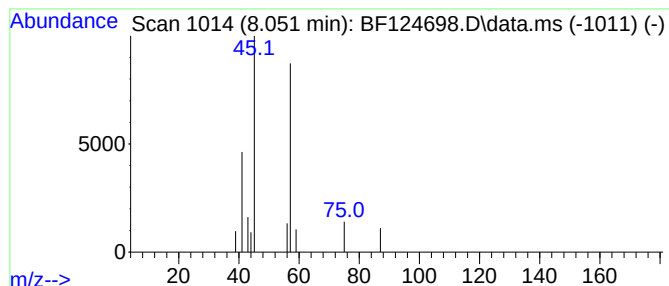
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Peak Number 2 unknown8.051 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	4.63 ng	9673	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Isobutoxymethyl)oxirane		130	C7H14O2		003814-55-9	9
2	di-tert-Butyl acetylenedicarboxy...		226	C12H18O4		066086-33-7	9
3	Aziridine, 1-(methoxymethyl)-		87	C4H9NO		001497-83-2	7
4	1-Pentanamine		87	C5H13N		000110-58-7	5
5	Neopentylamine		87	C5H13N		005813-64-9	5



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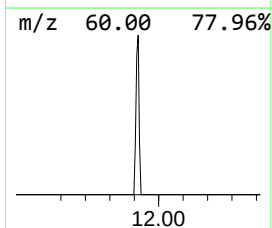
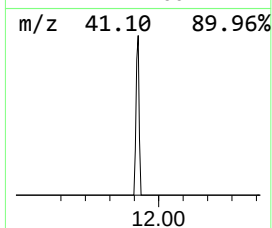
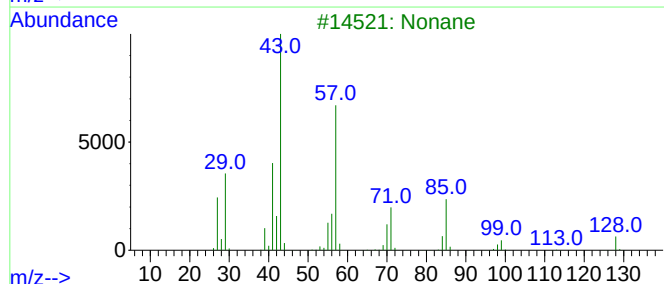
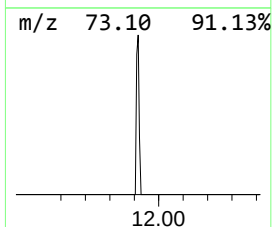
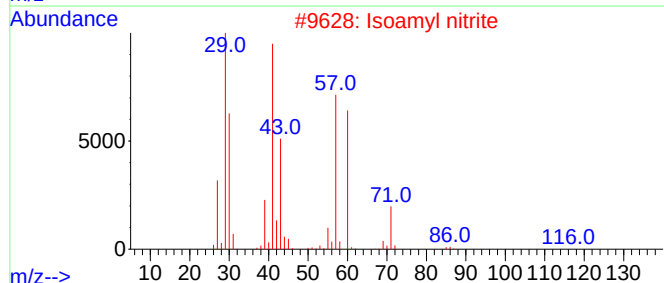
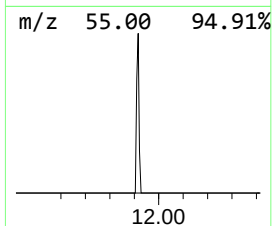
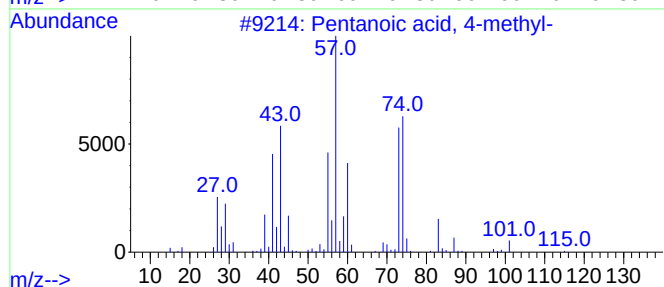
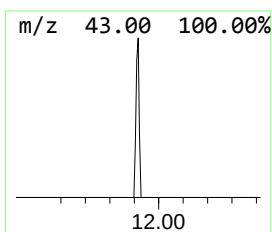
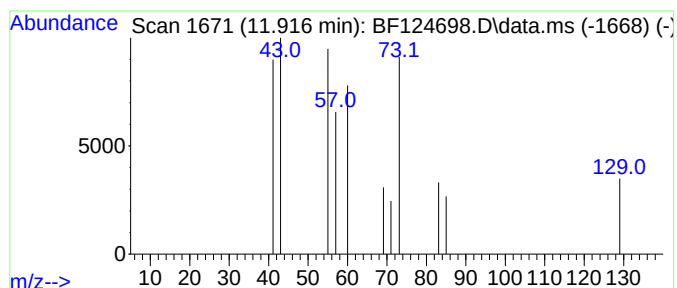
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Peak Number 3 unknown11.916 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.916	3.01 ng	6943	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-methyl-		116	C6H12O2	000646-07-1	9
2	Isoamyl nitrite		117	C5H11NO2	000110-46-3	9
3	Nonane		128	C9H20	000111-84-2	9
4	Octadecane, 1-(ethenyloxy)-		296	C20H40O	000930-02-9	9
5	1,6-Hexanediol		118	C6H14O2	000629-11-8	9



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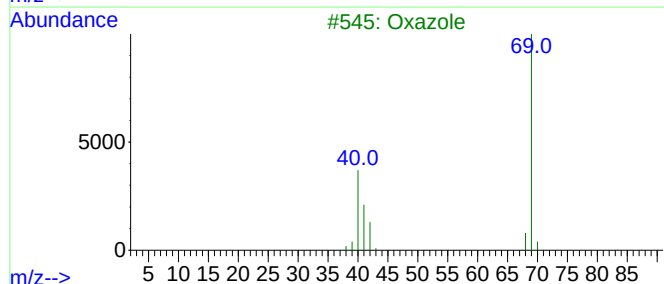
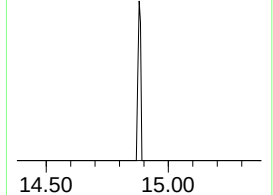
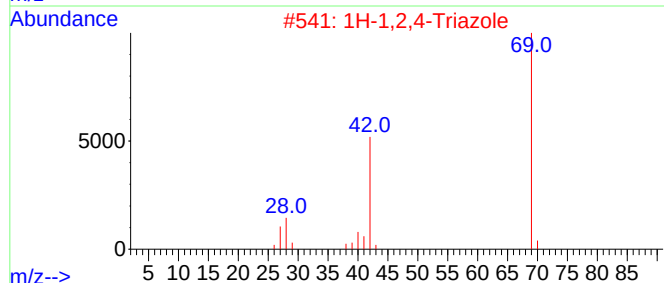
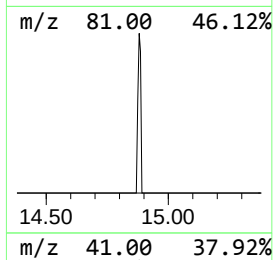
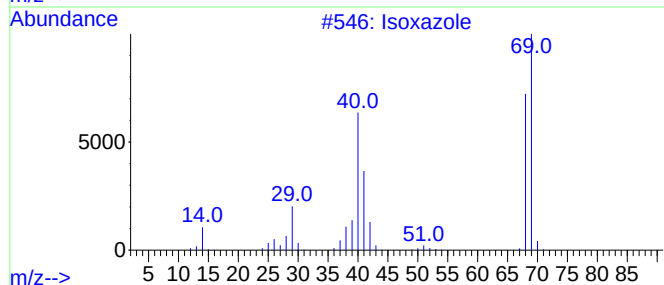
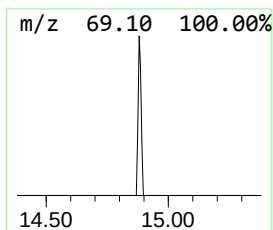
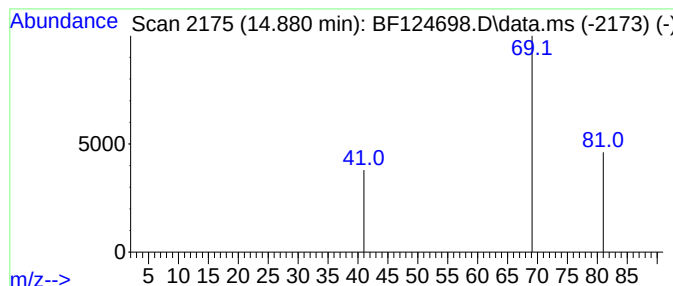
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Peak Number 4 unknown14.880 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.14 ng	3004	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoxazole	69	C3H3NO	000288-14-2	3
2			1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2
3			Oxazole	69	C3H3NO	000288-42-6	2
4			1H-1,2,3-Triazole	69	C2H3N3	000288-36-8	2
5			2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	10.2	ng	15227	1	6.869	29981	20.0
unknown8.051	8.051	4.6	ng	9673	2	8.151	41744	20.0
unknown11.916	11.916	3.0	ng	6943	4	11.392	46119	20.0
unknown14.880	14.880	2.1	ng	3004	6	15.498	28018	20.0