

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
 Data File : BF124678.D
 Acq On : 22 Jul 2021 1:43
 Operator : JU/CG
 Sample : M3076-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210587-AMENDED-COM-1

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-BF070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	20	rBB	10692	11705	6.75%	1.082%
2	5.110	509	514	518	rBB	16935	19860	11.45%	1.835%
3	5.504	576	581	583	rBB	130811	116344	67.06%	10.752%
4	6.510	747	752	754	rBB	145115	141247	81.41%	13.054%
5	6.887	813	816	819	rBB	44011	32961	19.00%	3.046%
6	7.451	907	912	914	rBB	106169	93946	54.15%	8.682%
7	8.069	1014	1017	1019	rBB	8125	5935	3.42%	0.549%
8	8.169	1031	1034	1037	rBB	58009	47229	27.22%	4.365%
9	9.245	1213	1217	1220	rBV	193964	173500	100.00%	16.035%
10	9.928	1330	1333	1336	rBB	73441	56033	32.30%	5.179%
11	10.716	1463	1467	1470	rBB	102339	82275	47.42%	7.604%
12	11.280	1561	1563	1566	rBB	6205	4565	2.63%	0.422%
13	11.416	1582	1586	1589	rBB	68178	54420	31.37%	5.029%
14	11.933	1671	1674	1676	rBB	10808	6564	3.78%	0.607%
15	12.721	1805	1808	1809	rBB	3146	2317	1.34%	0.214%
16	13.004	1851	1856	1859	rBB	186918	160242	92.36%	14.809%
17	13.892	2005	2007	2012	rBB2	4389	4833	2.79%	0.447%
18	14.051	2031	2034	2037	rBB	43563	34408	19.83%	3.180%
19	15.533	2281	2286	2289	rBV	29299	33647	19.39%	3.110%

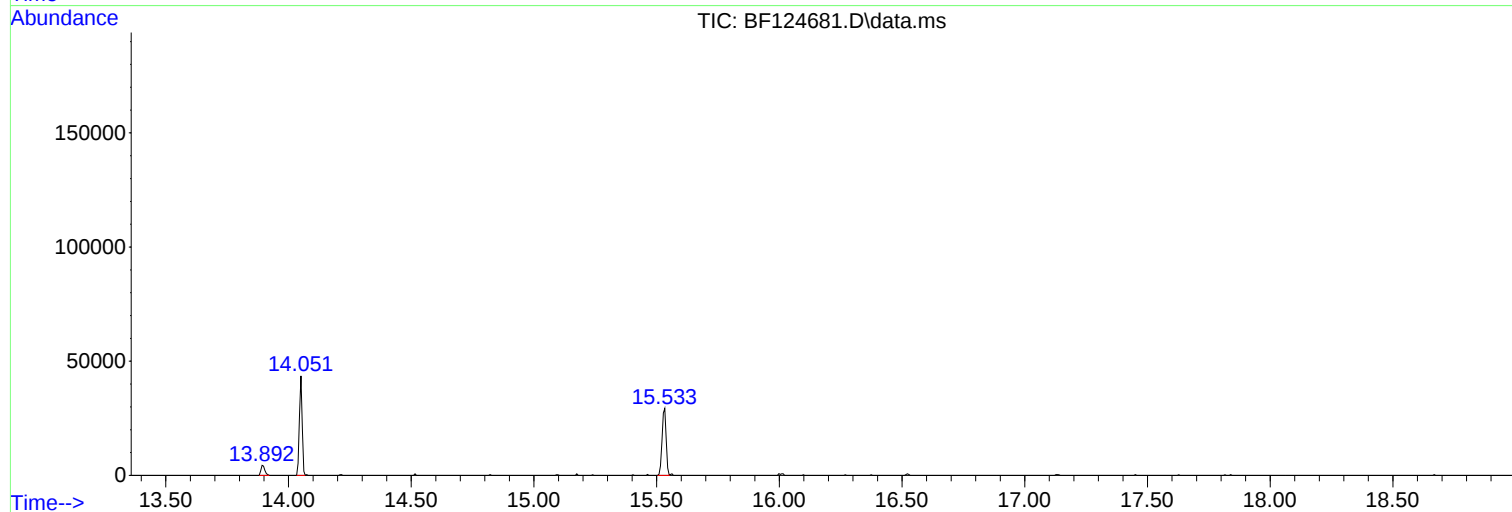
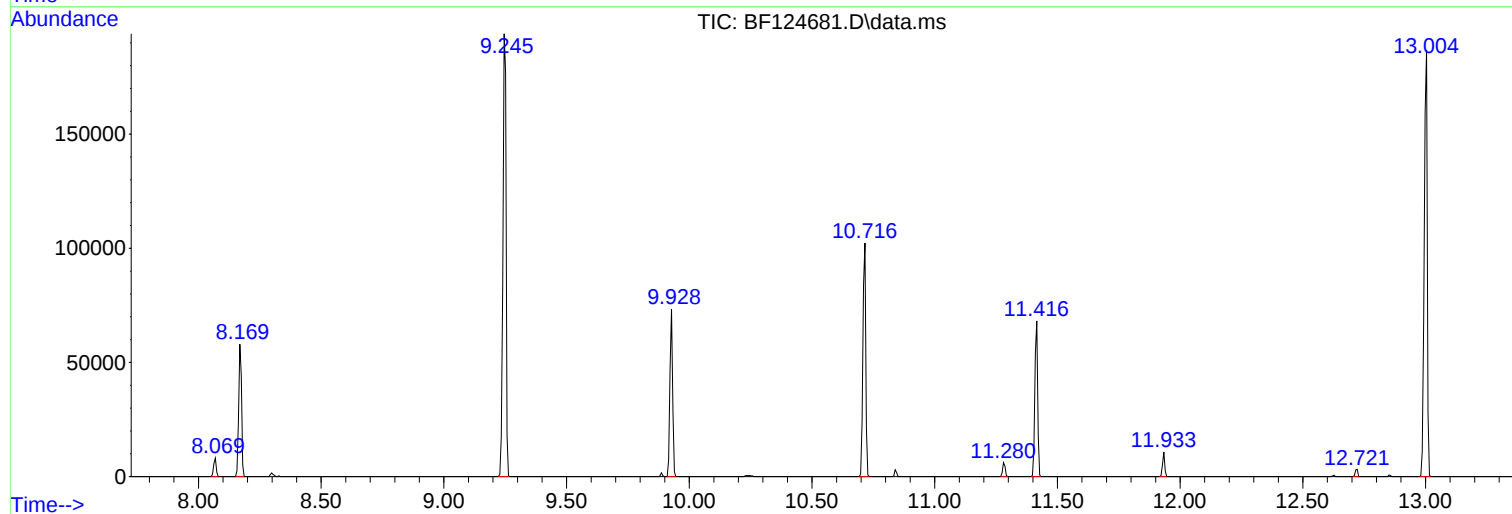
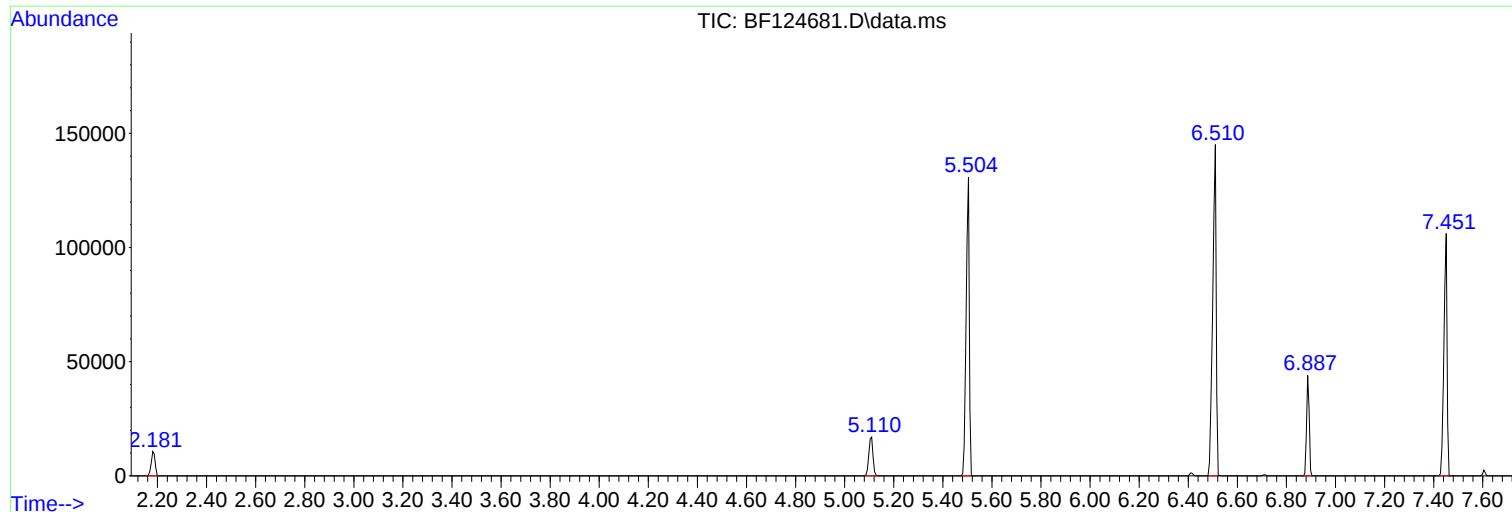
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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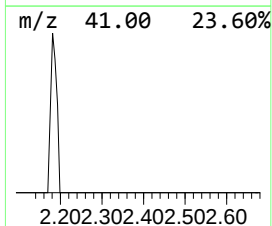
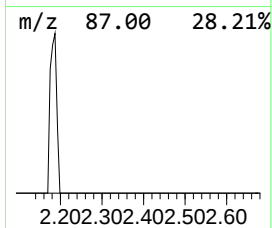
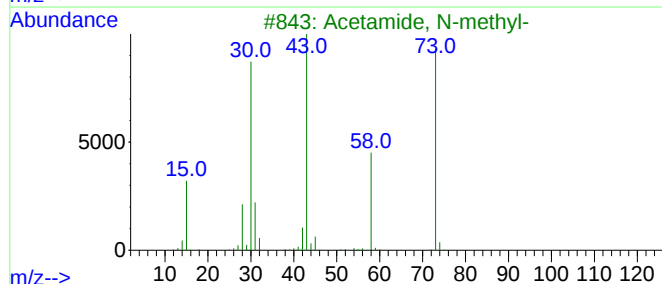
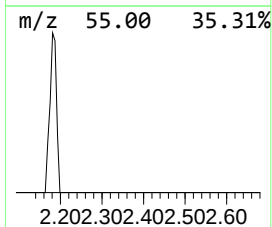
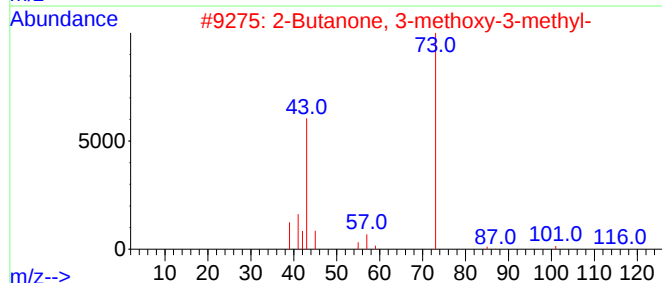
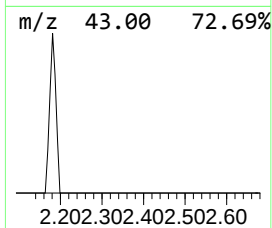
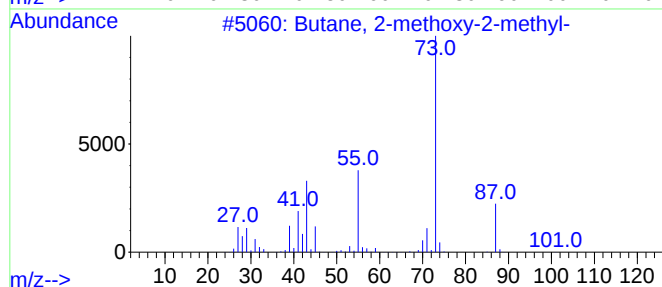
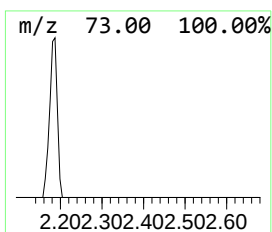
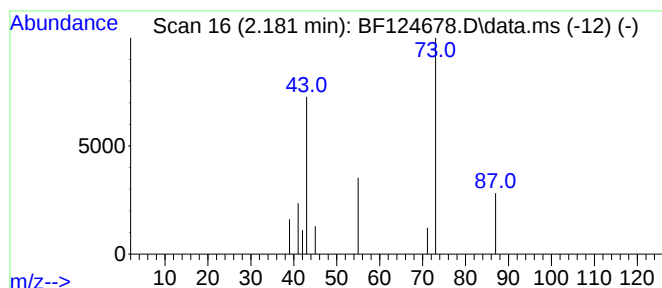
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	7.10 ng	11705	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			N-Ethylformamide	73	C3H7NO	000627-45-2	5



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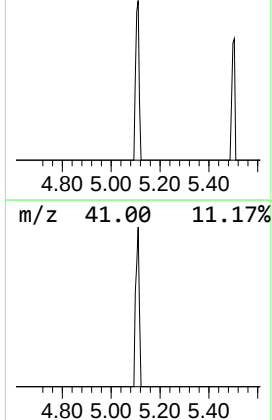
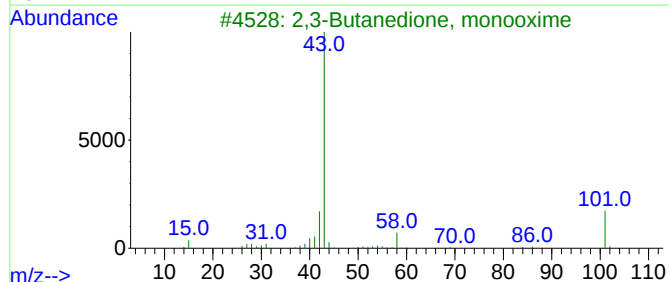
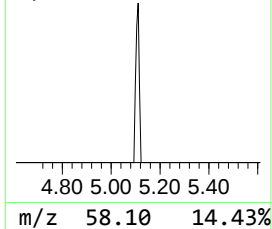
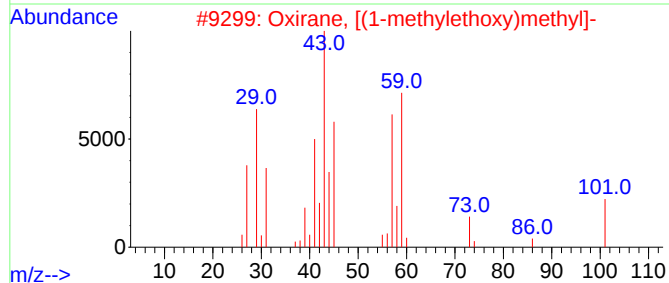
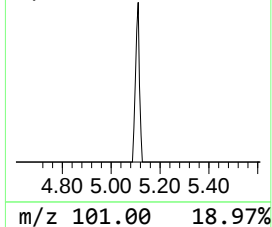
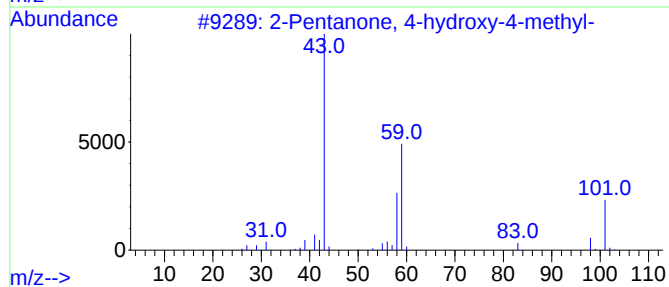
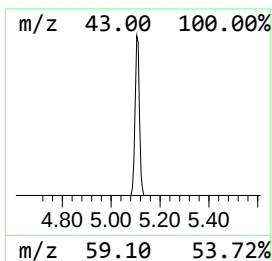
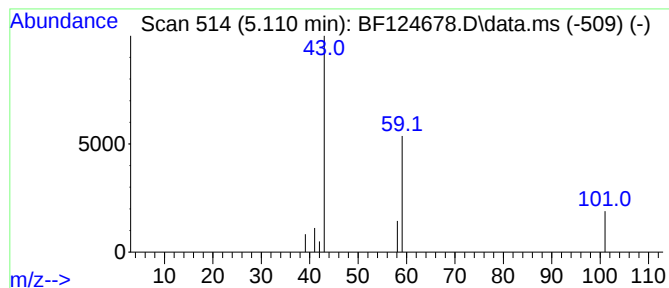
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	12.05 ng	19860	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
2			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
4			Diacetamide	101	C4H7NO2	000625-77-4	7
5			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	4



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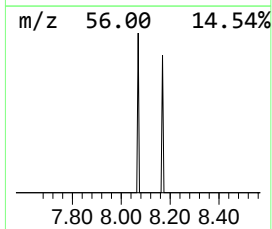
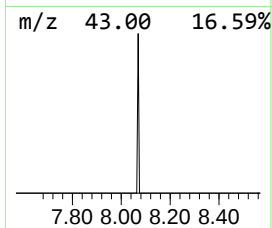
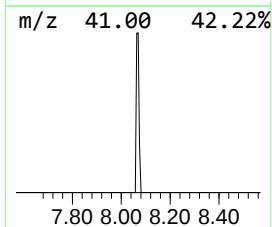
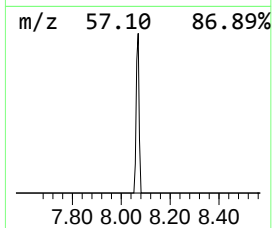
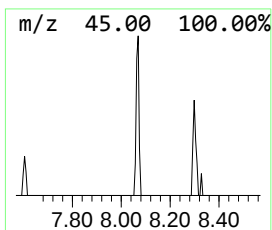
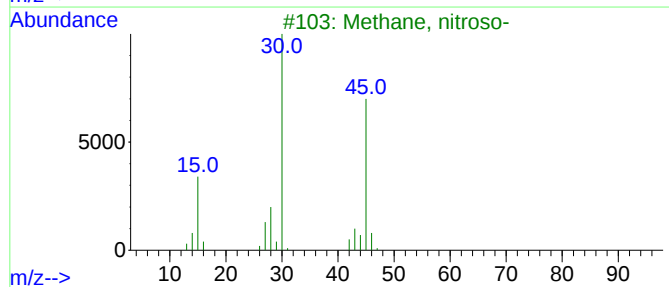
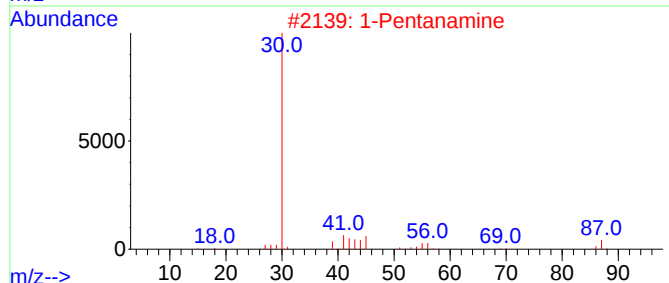
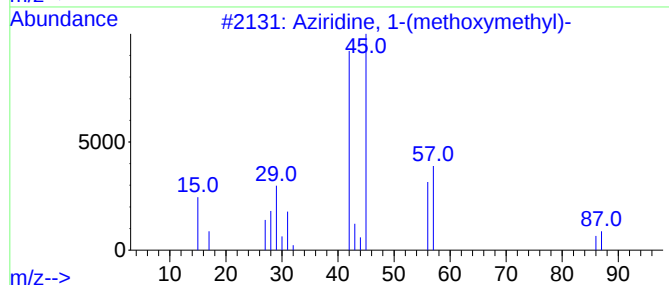
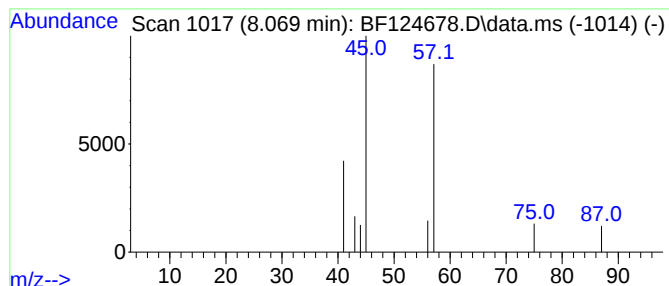
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Peak Number 3 unknown8.069 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.51 ng	5935	Naphthalene-d8	8.169

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7
2		1-Pentanamine	87	C5H13N	000110-58-7	5
3		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
5		Neopentylamine	87	C5H13N	005813-64-9	4



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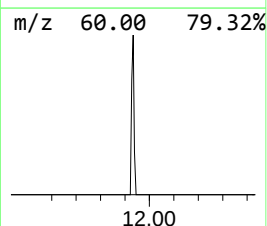
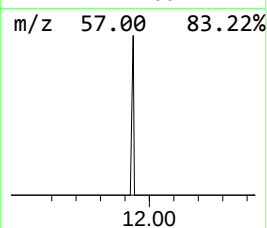
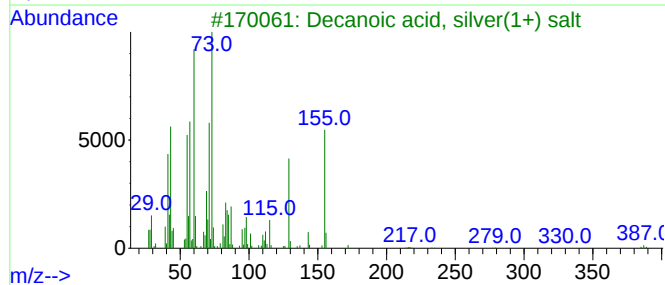
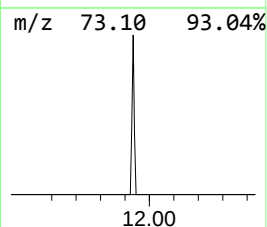
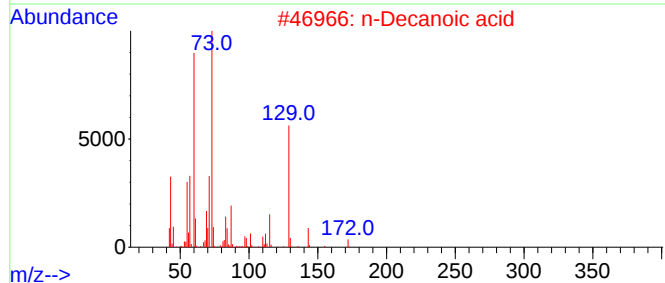
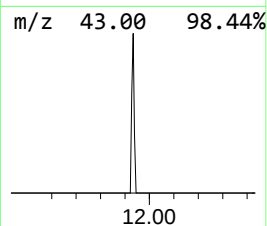
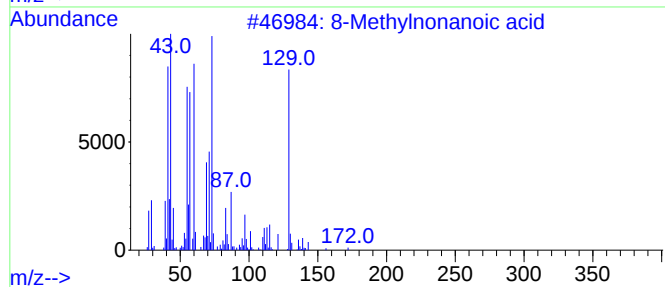
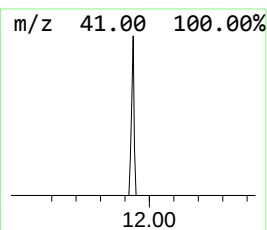
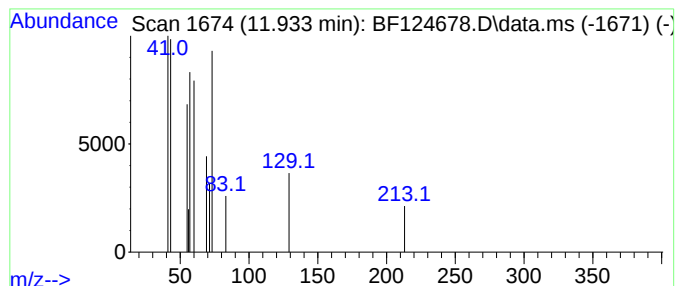
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Peak Number 4 8-Methylnonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.41 ng	6564	Phenanthrene-d10	11.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64
2		n-Decanoic acid	172	C10H20O2	000334-48-5	38
3		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	28
4		Amyl nitrite	117	C5H11NO2	000463-04-7	28
5		Dodecanoic acid	200	C12H24O2	000143-07-7	28



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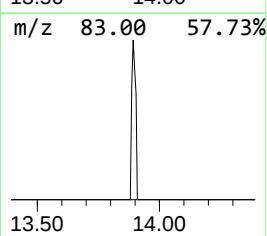
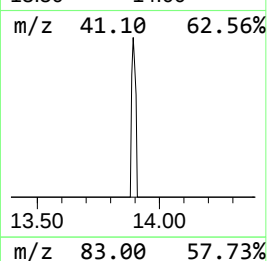
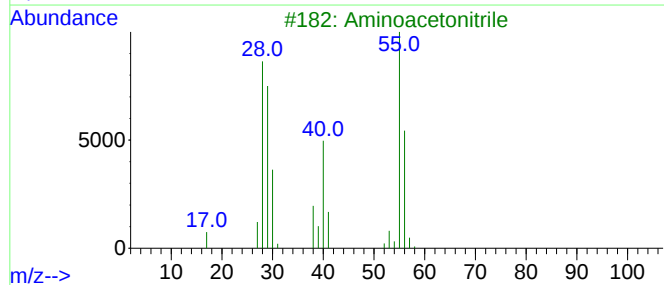
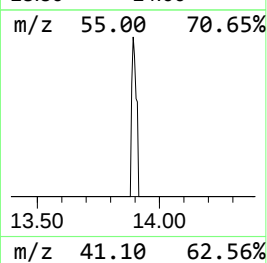
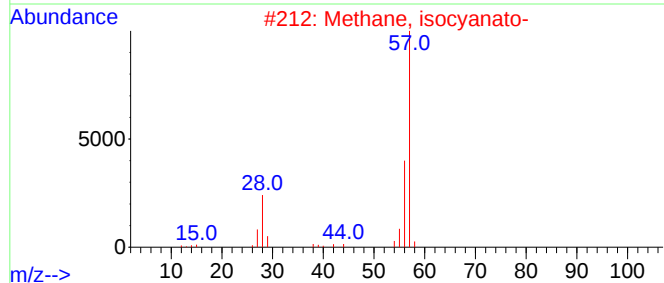
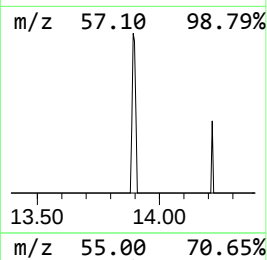
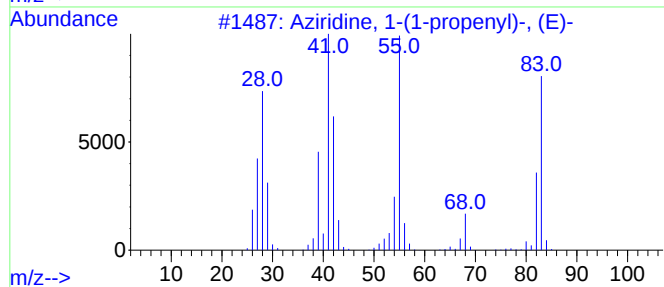
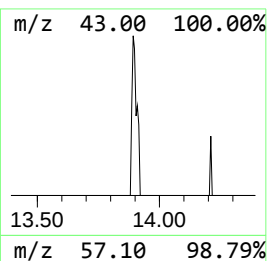
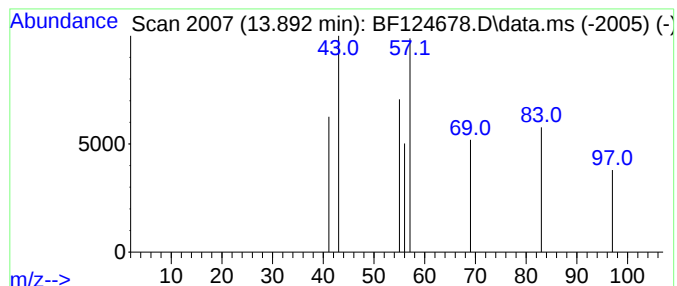
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Peak Number 5 unknown13.892 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	2.81 ng	4833	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
2			Methane, isocyanato-	57	C2H3NO	000624-83-9	4
3			Aminoacetonitrile	56	C2H4N2	000540-61-4	4
4			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
5			Azetidine	57	C3H7N	000503-29-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	7.1	ng	11705	1	6.887	32961	20.0
2-Pentanone, 4-...	5.110	12.1	ng	19860	1	6.887	32961	20.0
unknown8.069	8.069	2.5	ng	5935	2	8.169	47229	20.0
8-Methylnonanoi...	11.933	2.4	ng	6564	4	11.416	54420	20.0
unknown13.892	13.892	2.8	ng	4833	5	14.051	34408	20.0