

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
 Data File : BF131596.D
 Acq On : 12 Dec 2022 17:03
 Operator : CG\JU
 Sample : N5999-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-20

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	21	rVB	291218	364011	15.41%	2.405%
2	2.281	28	33	37	rVB	28428	34861	1.48%	0.230%
3	5.110	509	514	524	rVB	232634	313692	13.28%	2.073%
4	5.516	578	583	586	rBV	2113556	1987719	84.14%	13.133%
5	6.528	749	755	758	rBV	1937823	2028327	85.86%	13.401%
6	6.892	813	817	820	rVB	432444	346480	14.67%	2.289%
7	7.457	908	913	916	rBV	1229847	1311836	55.53%	8.667%
8	8.180	1031	1036	1039	rBV	500753	436966	18.50%	2.887%
9	9.263	1214	1220	1223	rBV	2669860	2362294	100.00%	15.607%
10	9.945	1332	1336	1339	rVB	644285	518005	21.93%	3.422%
11	10.745	1466	1472	1475	rBV	1730649	1665461	70.50%	11.004%
12	11.439	1586	1590	1594	rBV	625704	536539	22.71%	3.545%
13	11.968	1676	1680	1684	rBV	55414	47588	2.01%	0.314%
14	13.039	1857	1862	1865	rBV	2553390	2159511	91.42%	14.268%
15	13.998	2008	2025	2038	rBV5	76992	312307	13.22%	2.063%
16	14.098	2038	2042	2045	rVB	348924	326947	13.84%	2.160%
17	14.192	2053	2058	2062	rBV	63788	62613	2.65%	0.414%
18	15.609	2293	2299	2313	rBV	249320	320527	13.57%	2.118%

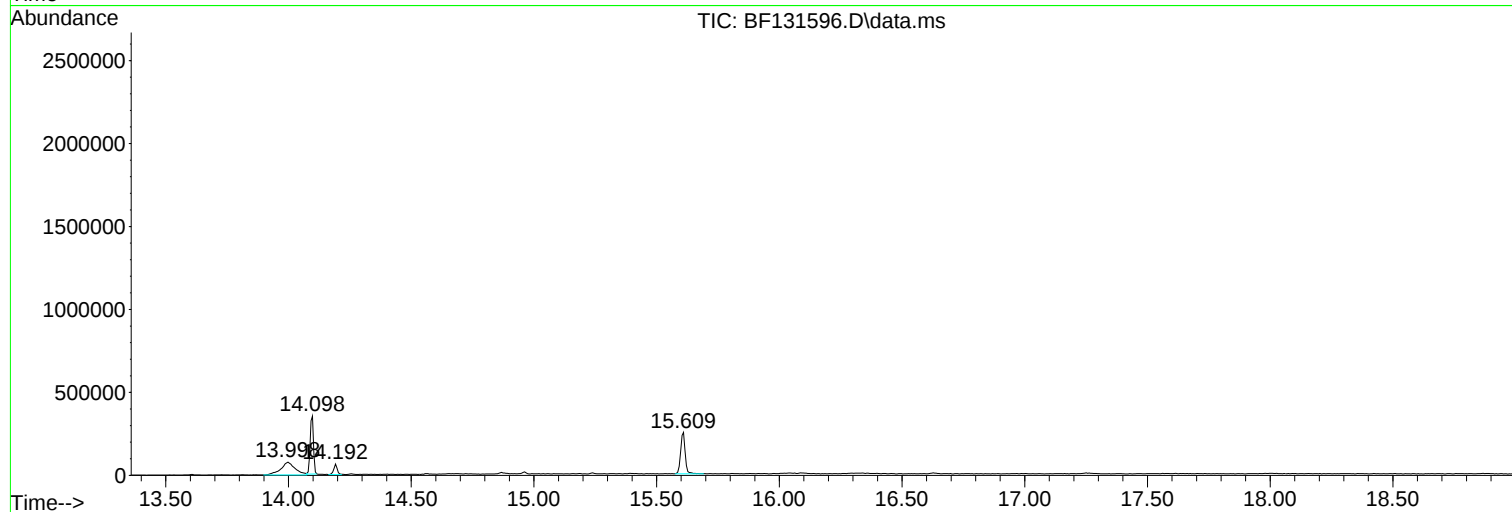
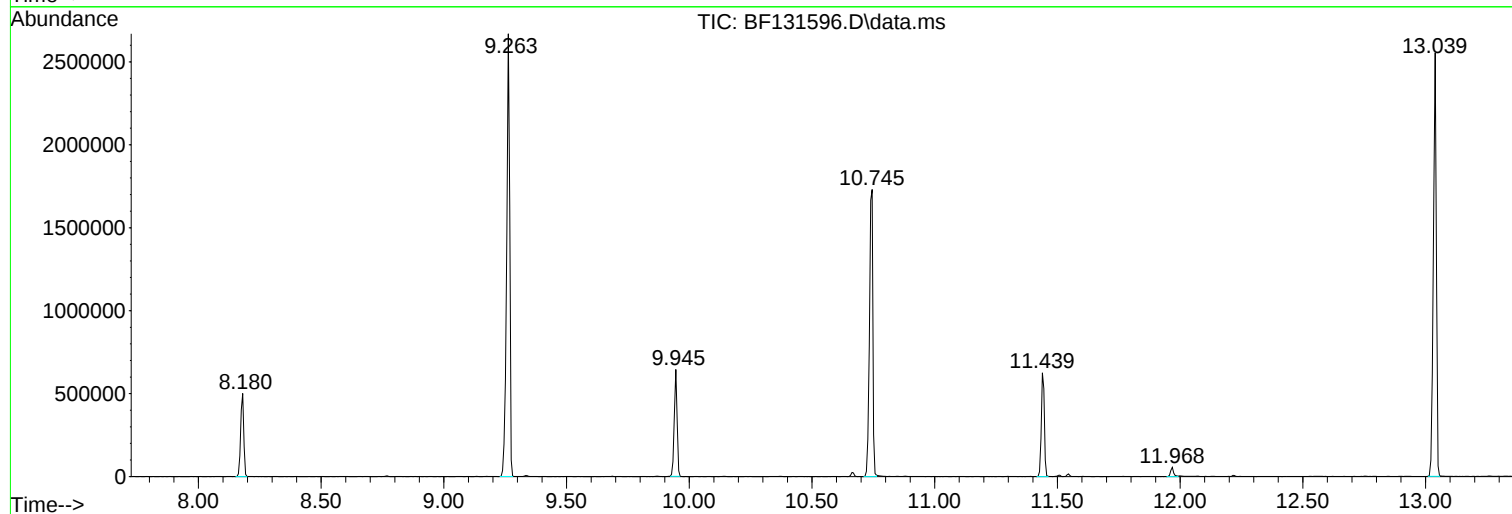
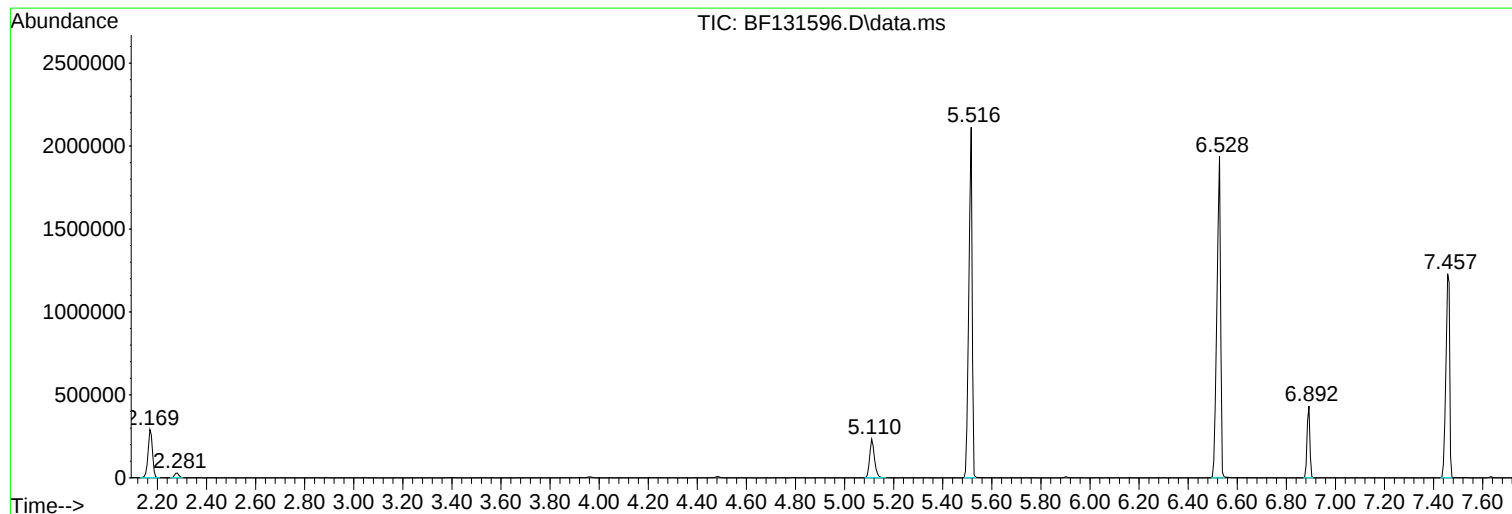
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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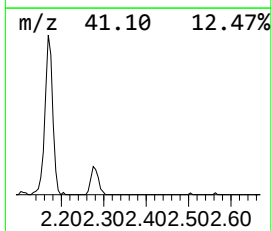
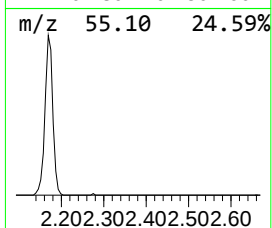
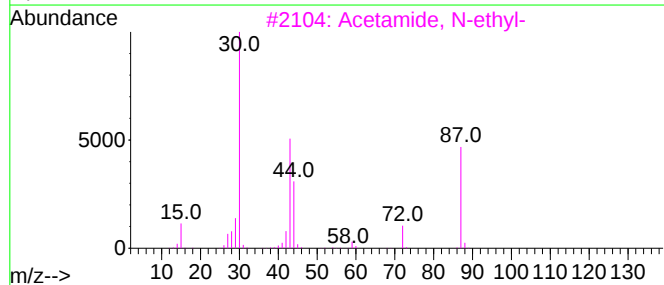
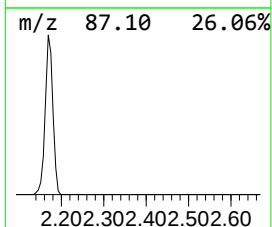
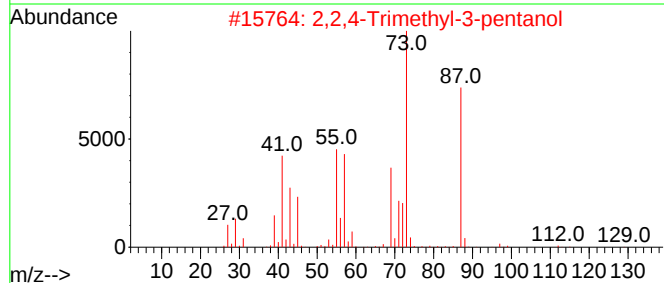
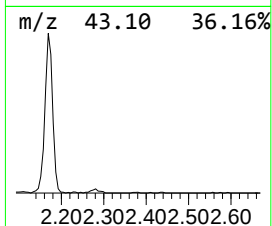
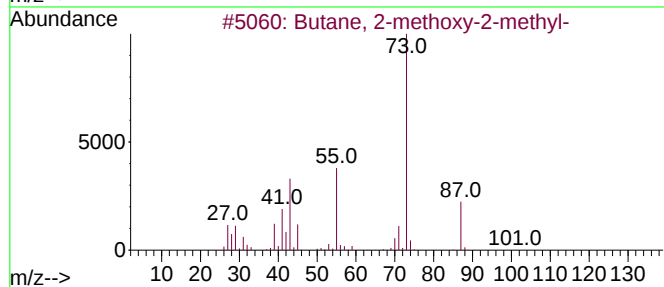
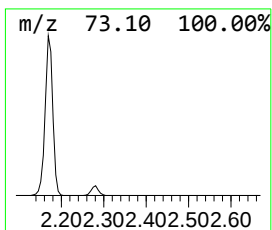
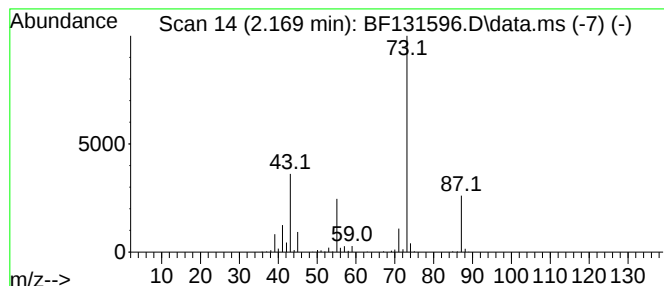
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.169	21.01 ng	364011	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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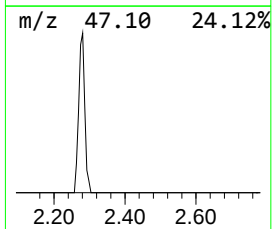
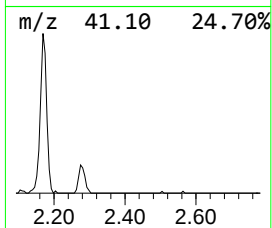
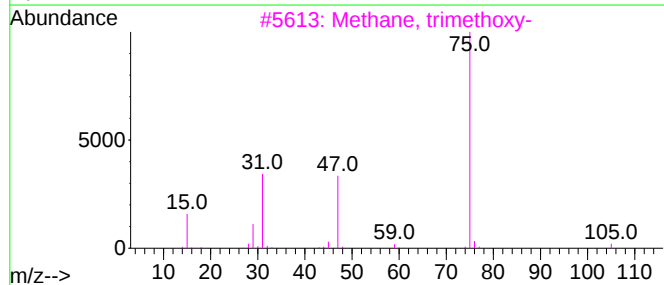
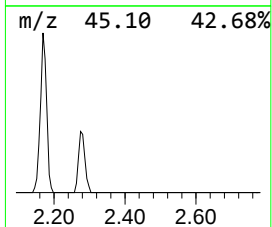
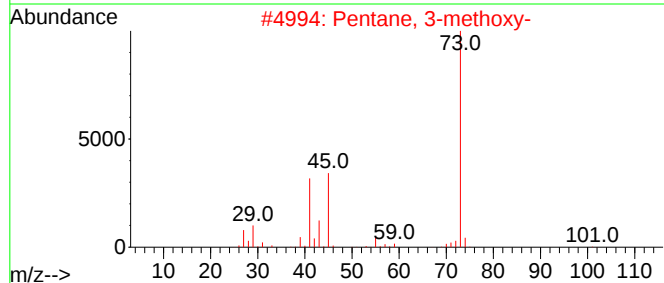
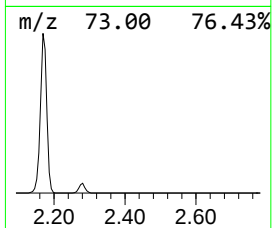
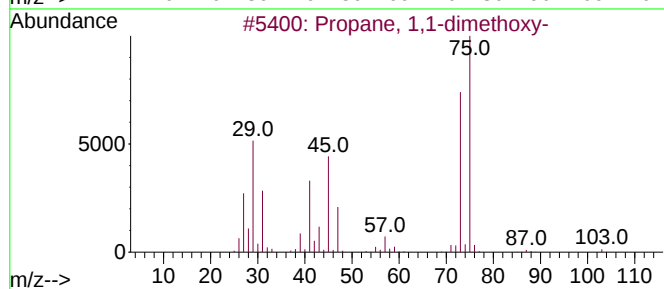
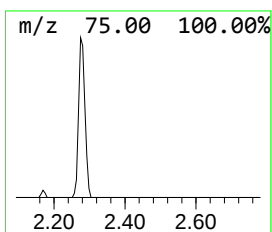
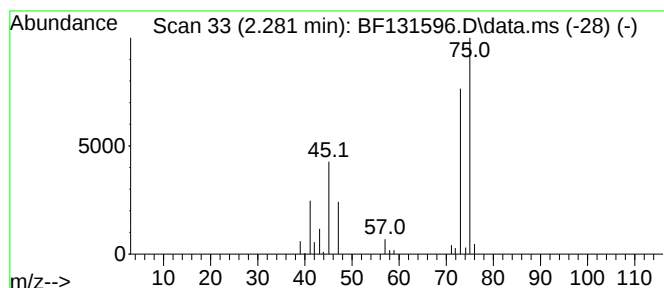
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.01 ng	34861	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3			Methane, trimethoxy-	106	C4H10O3	000149-73-5	9
4			Glycine	75	C2H5NO2	000056-40-6	7
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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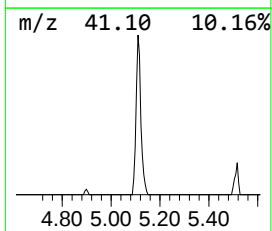
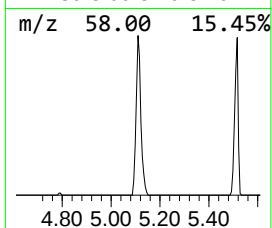
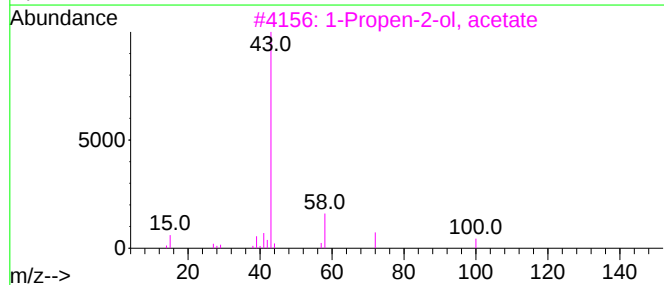
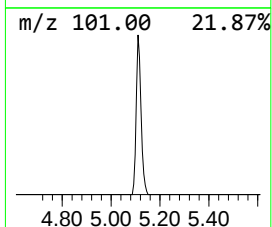
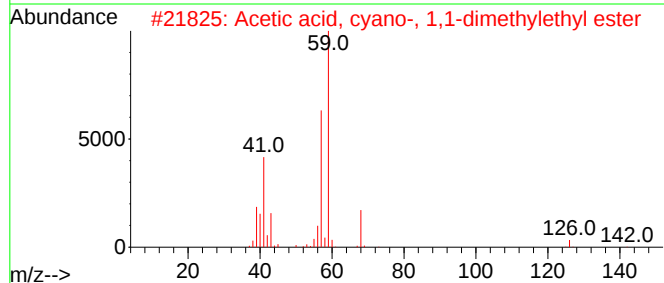
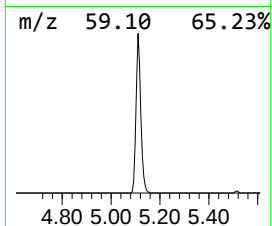
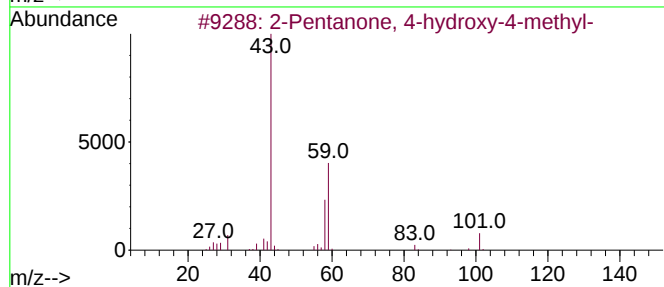
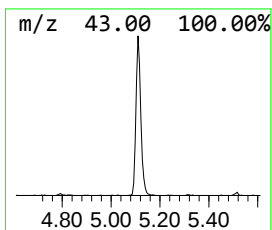
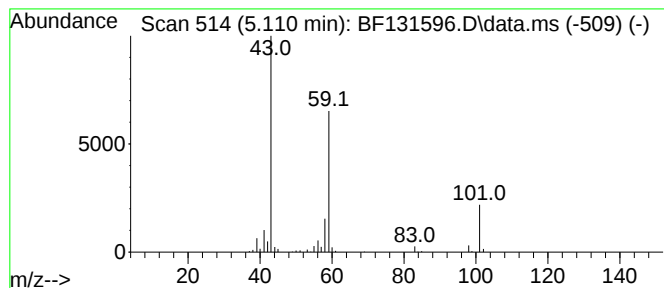
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	18.11 ng	313692	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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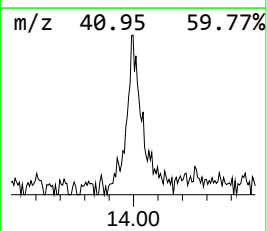
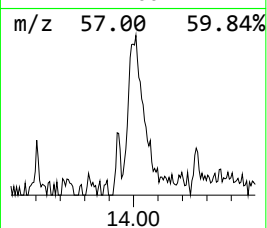
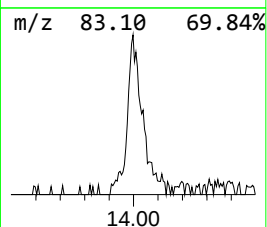
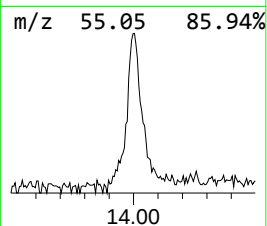
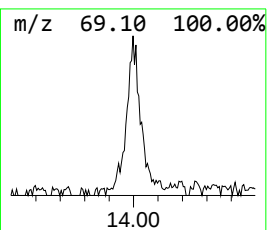
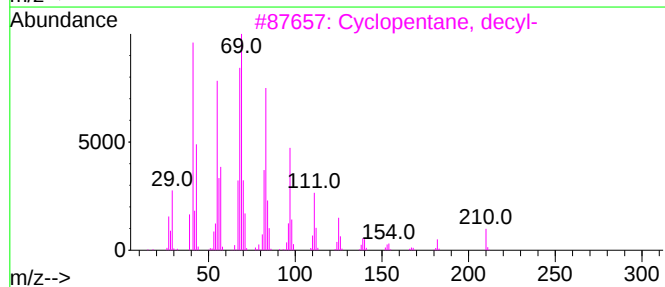
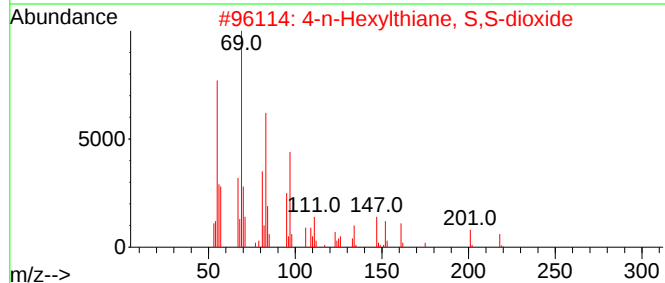
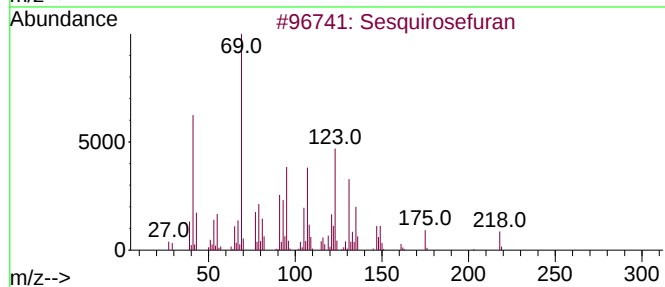
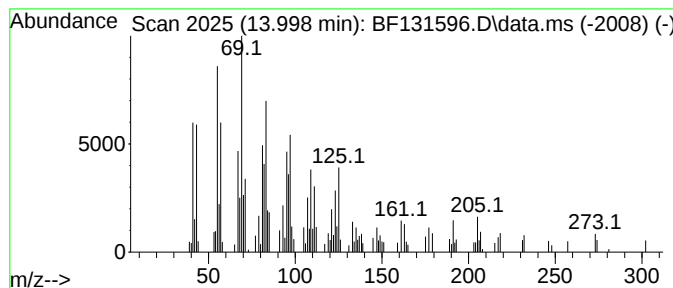
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Peak Number 4 Sesquirosefuran Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	19.10 ng	312307	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sesquirosefuran	218	C15H22O	039007-93-7	90
2			4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	46
3			Cyclopentane, decyl-	210	C15H30	001795-21-7	43
4			4-n-Pentylthiane, S,S-dioxide	204	C10H20O2S	065865-33-0	38
5			Eicosyl methyl ether	312	C21H44O	1000406-29-4	35



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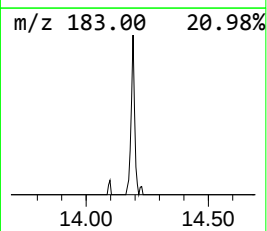
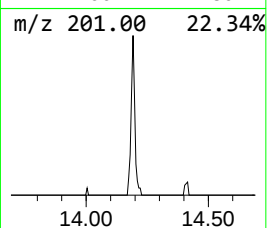
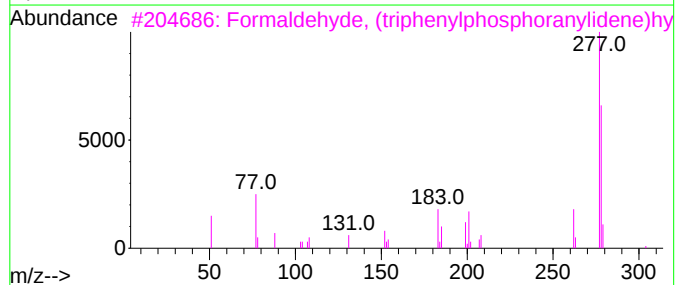
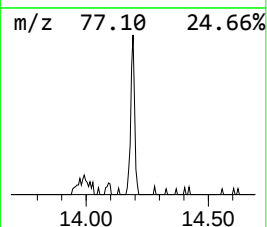
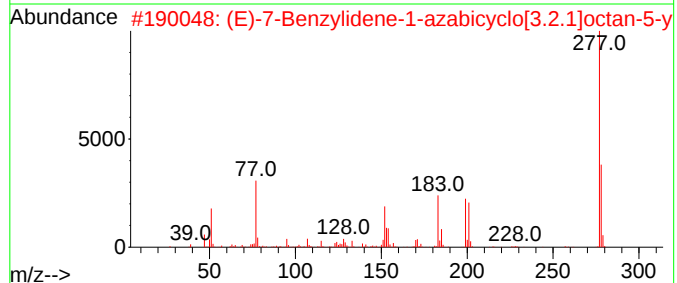
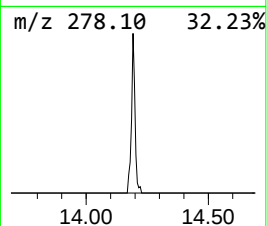
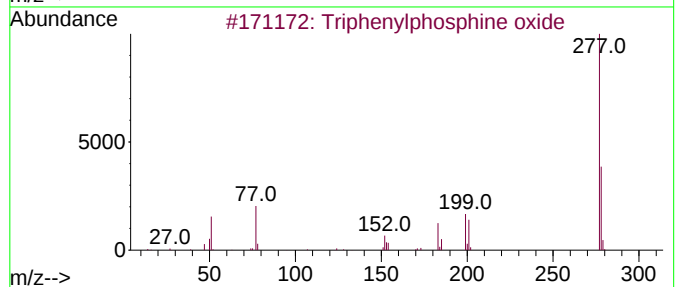
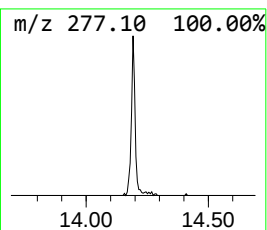
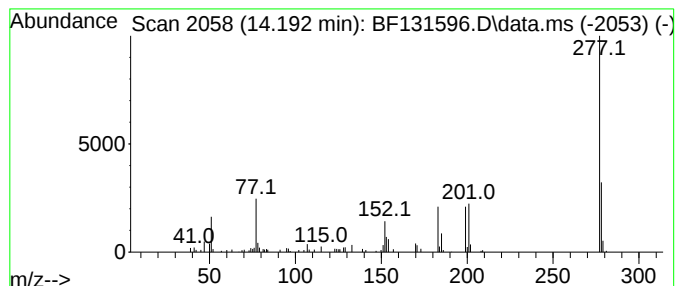
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.83 ng	62613	Chrysene-d12	14.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	40
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	25
5			1H-Indole-3-acetic acid, 5-[(tri...]	277	C14H19N03Si	072101-35-0	17



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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...	2.169	21.0	ng	364011	1	6.892	346480	20.0
Propane, 1,1-di...	2.281	2.0	ng	34861	1	6.892	346480	20.0
2-Pentanone, 4-...	5.110	18.1	ng	313692	1	6.892	346480	20.0
Sesquirosefuran	13.998	19.1	ng	312307	5	14.098	326947	20.0
Triphenylphosph...	14.192	3.8	ng	62613	5	14.098	326947	20.0