

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110122\
 Data File : BF130899.D
 Acq On : 01 Nov 2022 14:16
 Operator : CG\JU
 Sample : N5336-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-16.5-17.0

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	25	32	38	rVB	603144	774854	28.57%	4.232%
2	5.169	519	524	532	rVB	275724	341169	12.58%	1.863%
3	5.557	584	590	593	rBV	2226848	2139865	78.89%	11.686%
4	6.551	753	759	762	rBV	1979607	2280342	84.07%	12.454%
5	6.934	820	824	827	rBV	664991	539710	19.90%	2.948%
6	7.498	914	920	923	rBV	1443482	1485123	54.75%	8.111%
7	8.116	1021	1025	1037	rBV	40809	89741	3.31%	0.490%
8	8.216	1037	1042	1046	rVV	809273	729345	26.89%	3.983%
9	9.298	1220	1226	1229	rBV	3059433	2712496	100.00%	14.814%
10	9.980	1336	1342	1345	rBV	1067465	904714	33.35%	4.941%
11	10.774	1472	1477	1480	rBV	1921898	1794532	66.16%	9.800%
12	11.474	1592	1596	1599	rBV	1109472	904401	33.34%	4.939%
13	11.539	1602	1607	1610	rVB2	42480	39630	1.46%	0.216%
14	11.986	1678	1683	1687	rBV	43809	39528	1.46%	0.216%
15	13.063	1862	1866	1869	rBV	2592501	2364749	87.18%	12.915%
16	14.027	2022	2030	2042	rBV8	37209	165330	6.10%	0.903%
17	14.121	2042	2046	2049	rVB	556525	499021	18.40%	2.725%
18	14.215	2057	2062	2067	rBV	50160	59814	2.21%	0.327%
19	15.633	2298	2303	2313	rVB2	327902	446262	16.45%	2.437%

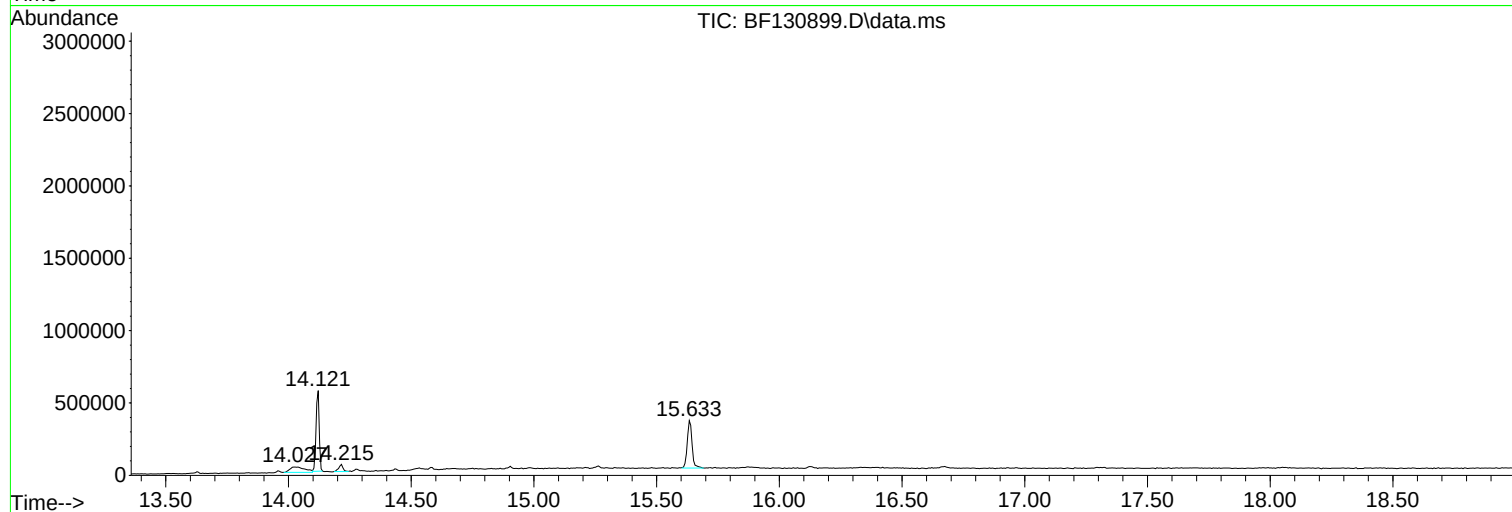
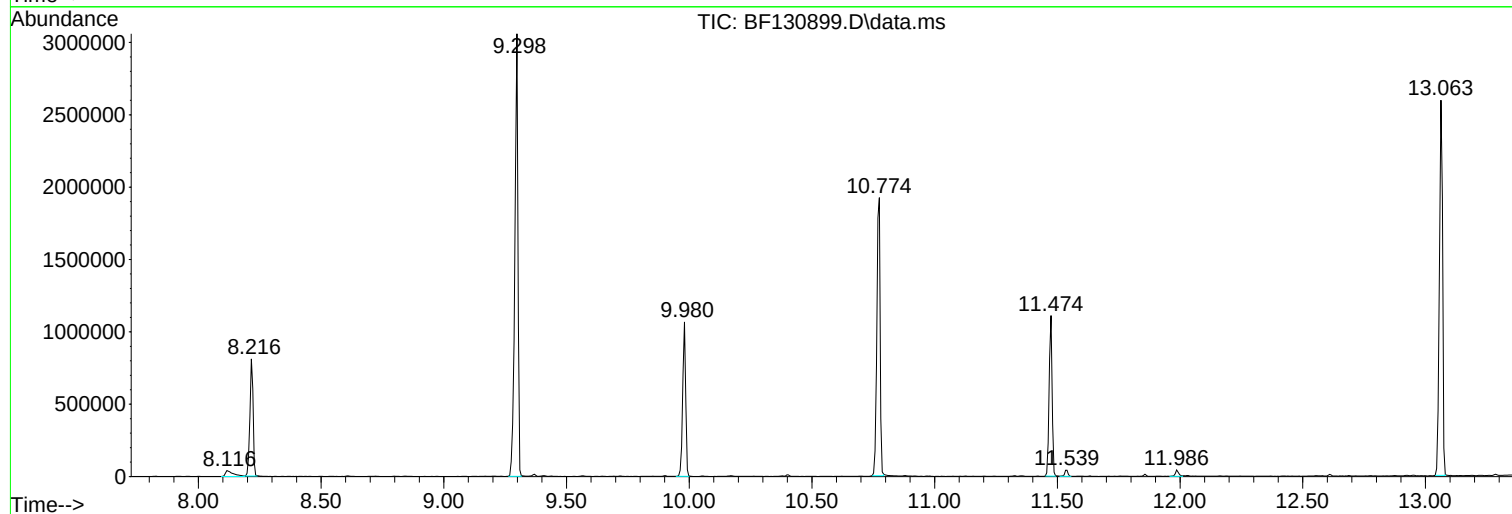
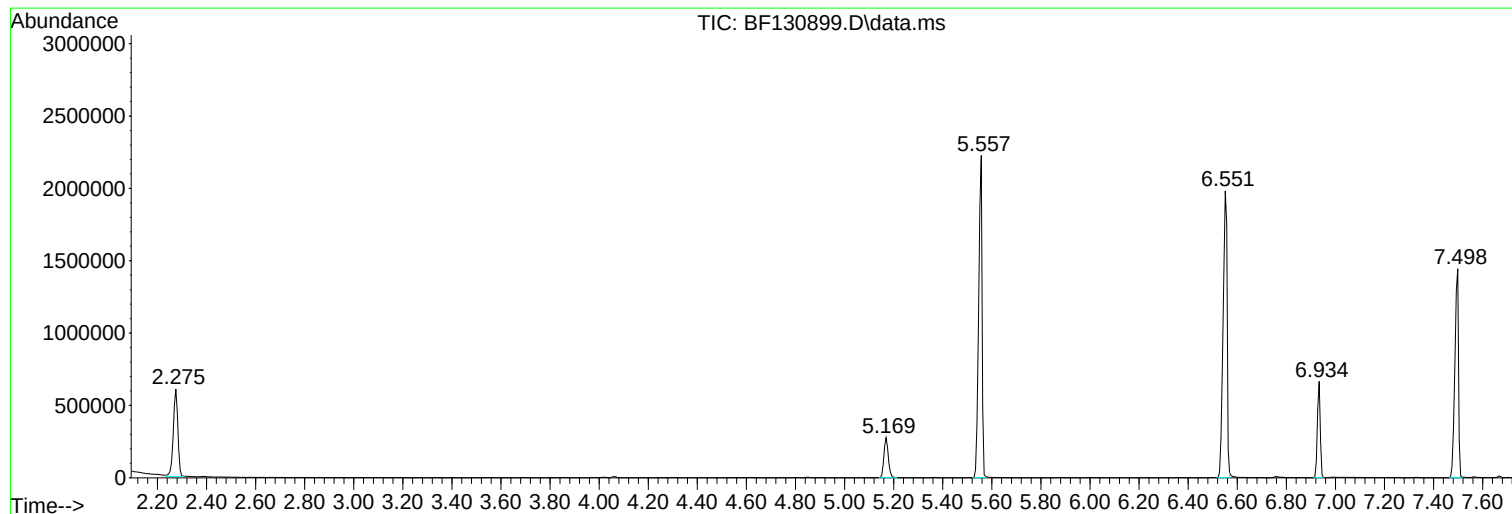
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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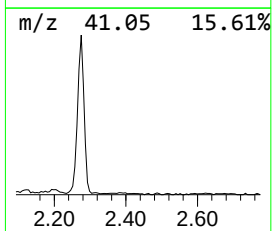
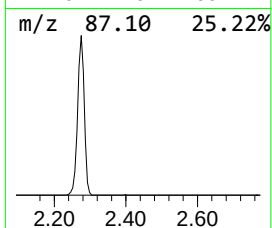
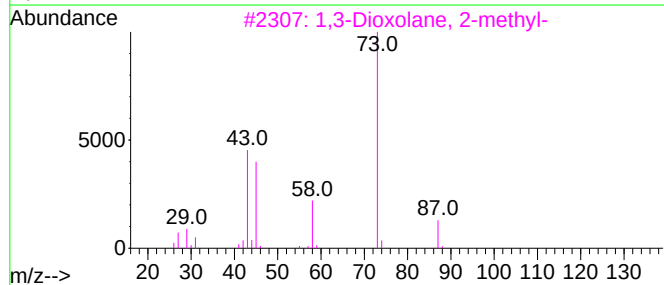
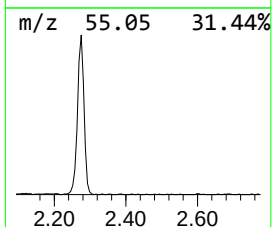
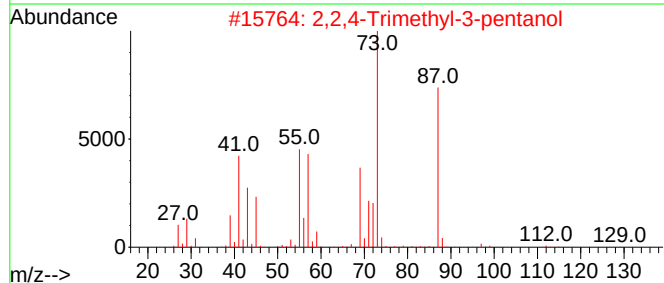
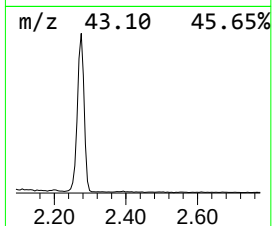
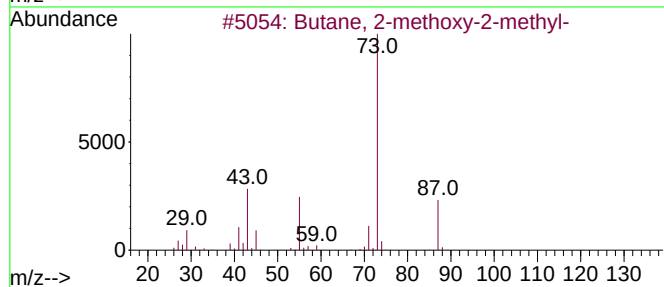
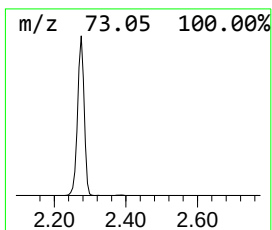
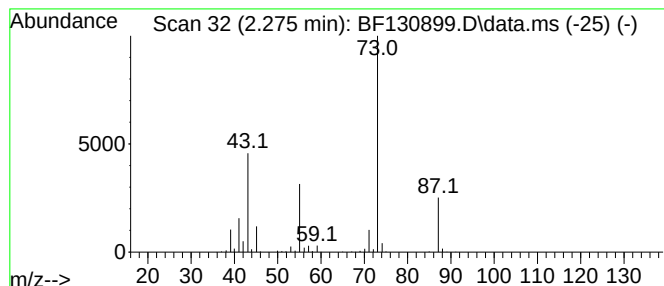
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.275	28.71 ng	774854	1,4-Dichlorobenzene-d4	6.934

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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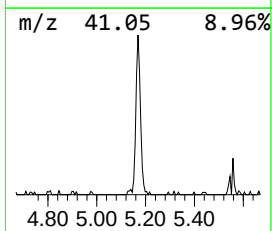
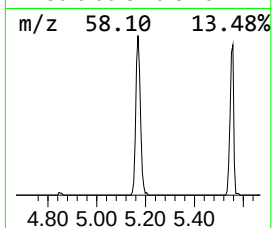
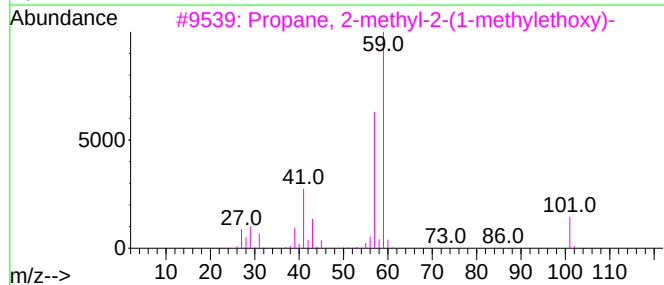
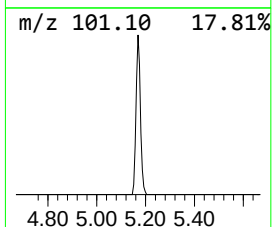
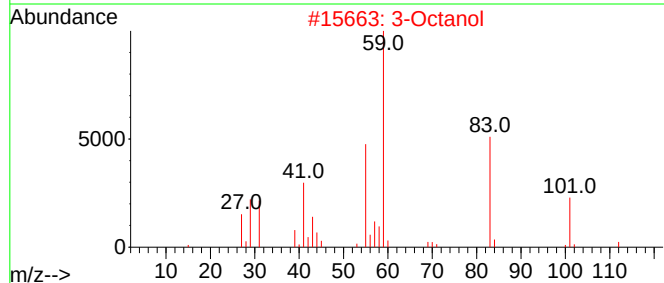
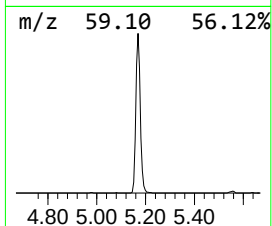
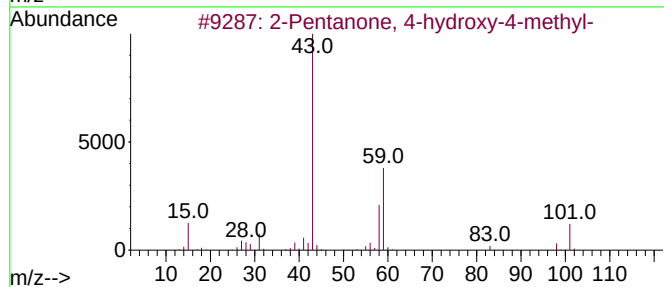
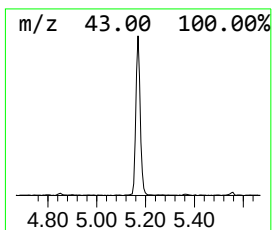
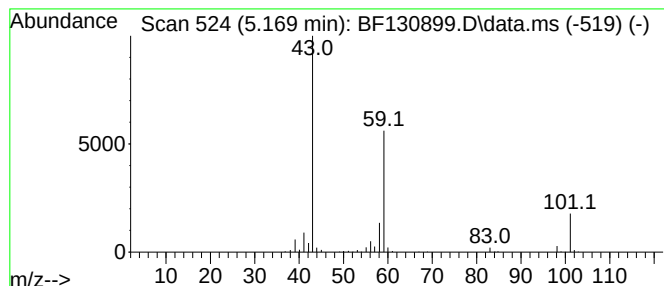
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.169	12.64 ng	341169	1,4-Dichlorobenzene-d4			6.934
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	3-Octanol		130	C8H18O	000589-98-0	36
3	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12



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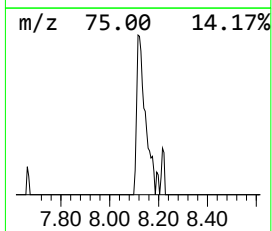
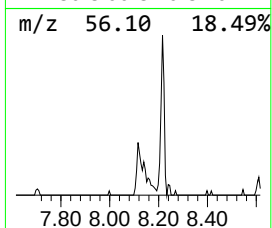
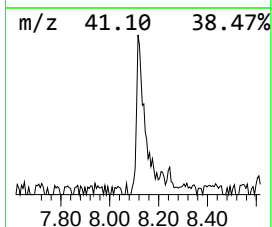
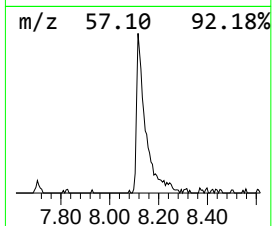
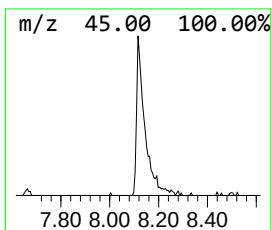
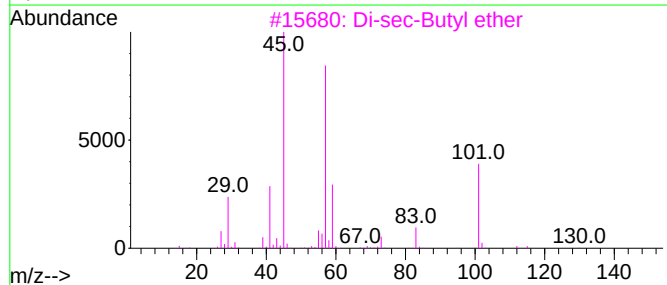
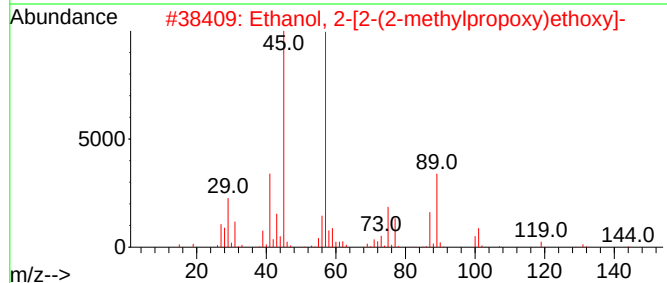
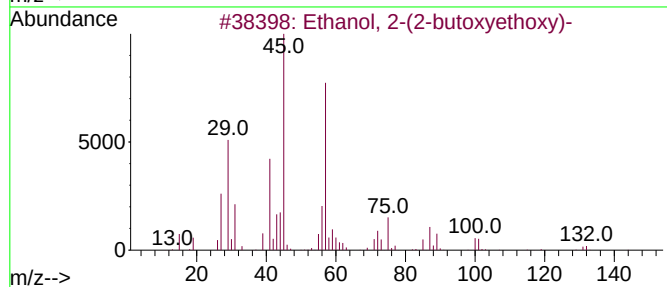
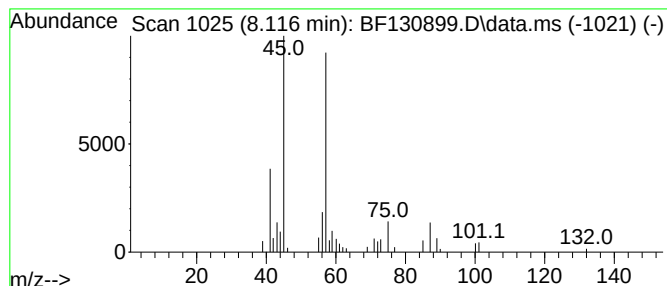
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	2.46 ng	89741	Naphthalene-d8	8.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
5			3,6,9,12-Tetraoxatetradeca-1,13-...	202	C10H18O4	000765-12-8	45



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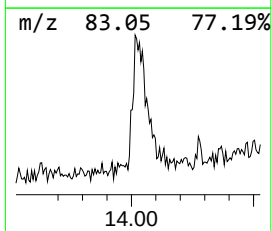
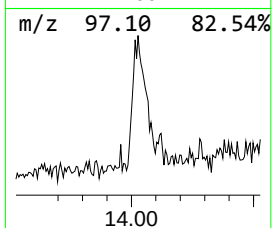
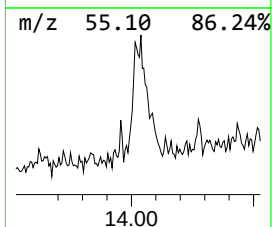
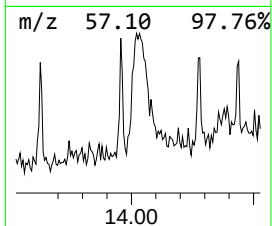
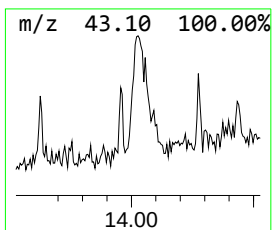
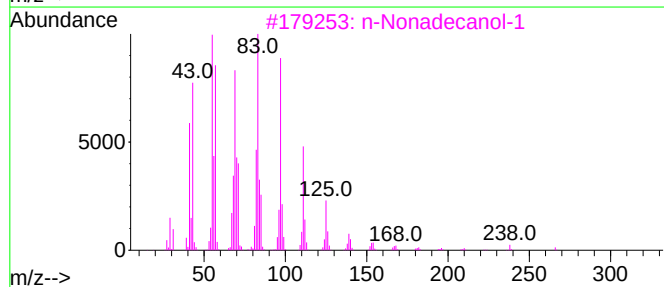
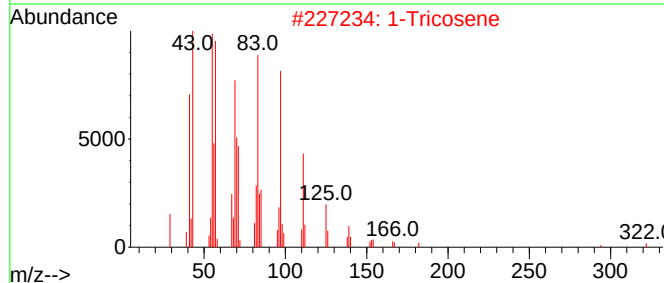
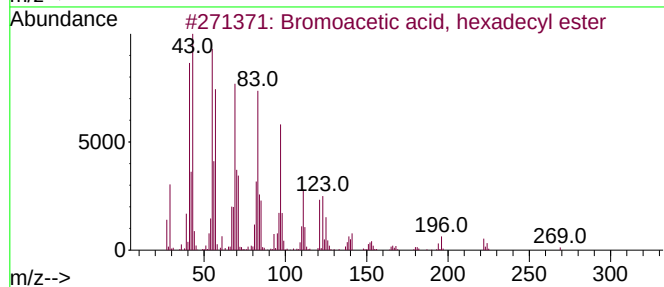
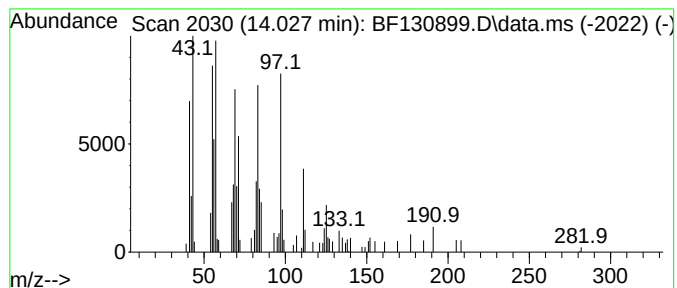
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Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	6.63 ng	165330	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2			1-Tricosene	322	C23H46	018835-32-0	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4			1-Heneicosanol	312	C21H44O	015594-90-8	90
5			Behenic alcohol	326	C22H46O	000661-19-8	90



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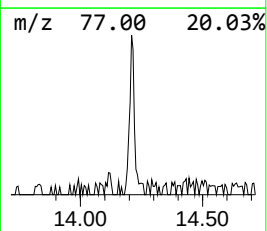
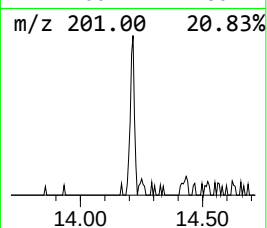
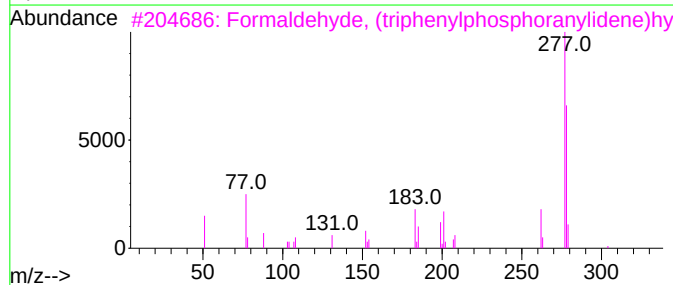
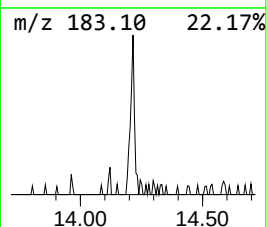
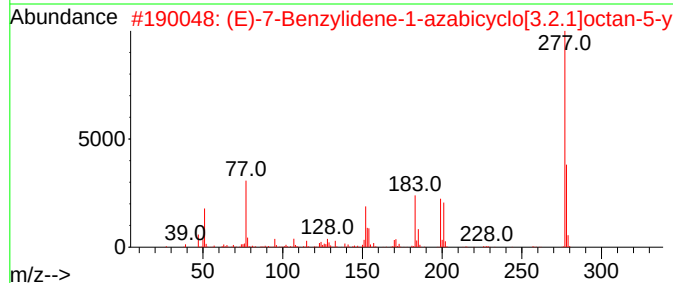
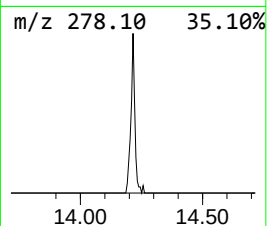
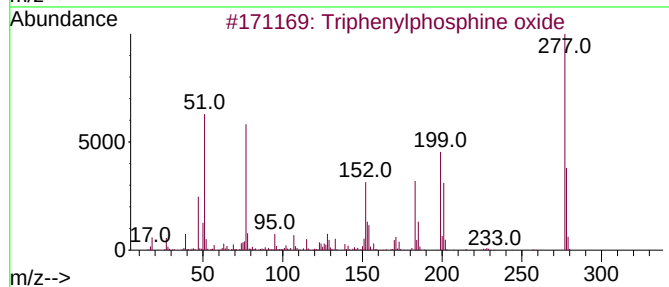
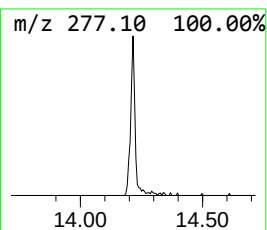
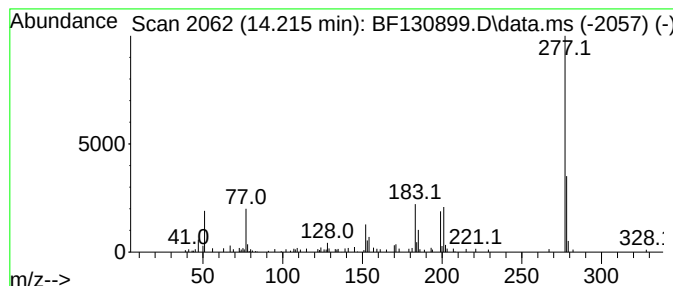
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.215	2.40 ng	59814	Chrysene-d12	14.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3.1.0]hex-2-ene	293	C15H19N03S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphoranylidene)hy	304	C19H17N2P	015990-54-2	59
4			Vanadium, cycloheptatrienyl-(pen...)	277	C17H22V	1000155-20-5	47
5			Cobalt, (.eta.<5>-2,4-cyclopentadienyl)-	277	C16H15BCo	036682-12-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.275	28.7	ng	774854	1	6.934	539710	20.0
2-Pentanone, 4-...	5.169	12.6	ng	341169	1	6.934	539710	20.0
Ethanol, 2-(2-b...	8.116	2.5	ng	89741	2	8.216	729345	20.0
Bromoacetic aci...	14.027	6.6	ng	165330	5	14.121	499021	20.0
Triphenylphosph...	14.215	2.4	ng	59814	5	14.121	499021	20.0