

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
 Data File : BF131570.D
 Acq On : 09 Dec 2022 17:03
 Operator : CG\JU
 Sample : N5911-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A3594TOG

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: BF131570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	14	21	26	rBV	1738795	2180886	17.79%	6.743%
2	5.116	511	515	523	rVB	264064	297933	2.43%	0.921%
3	5.516	578	583	586	rBV	1007970	873362	7.13%	2.700%
4	6.522	750	754	762	rBV	649516	565027	4.61%	1.747%
5	6.904	815	819	823	rBV	453699	409486	3.34%	1.266%
6	6.969	827	830	840	rBV	85397	159340	1.30%	0.493%
7	7.481	908	917	920	rBV	1536595	1703353	13.90%	5.267%
8	8.198	1034	1039	1045	rVB	618133	602435	4.91%	1.863%
9	9.280	1217	1223	1226	rBV	3731686	3269160	26.67%	10.108%
10	9.957	1334	1338	1342	rBV	650913	603352	4.92%	1.865%
11	10.757	1467	1474	1477	rBV	2103776	1986313	16.20%	6.141%
12	11.404	1574	1584	1587	rBV	936818	1739619	14.19%	5.379%
13	11.451	1589	1592	1596	rVB	709604	633618	5.17%	1.959%
14	11.621	1617	1621	1624	rVB	2602726	2172142	17.72%	6.716%
15	12.045	1681	1693	1695	rBV	8707068	12257516	100.00%	37.899%
16	13.051	1859	1864	1867	rBV	1919979	1815207	14.81%	5.612%
17	14.104	2039	2043	2049	rVB	584566	520140	4.24%	1.608%
18	14.198	2055	2059	2068	rBV	147530	141016	1.15%	0.436%
19	15.615	2294	2300	2309	rVB	334988	412775	3.37%	1.276%

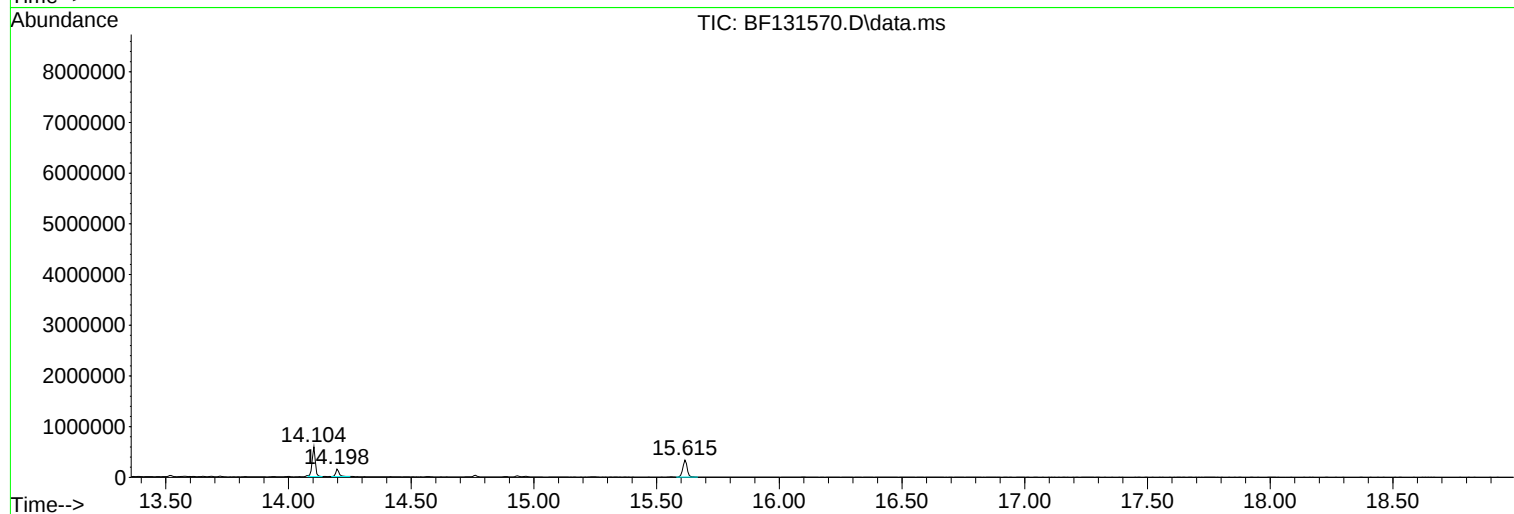
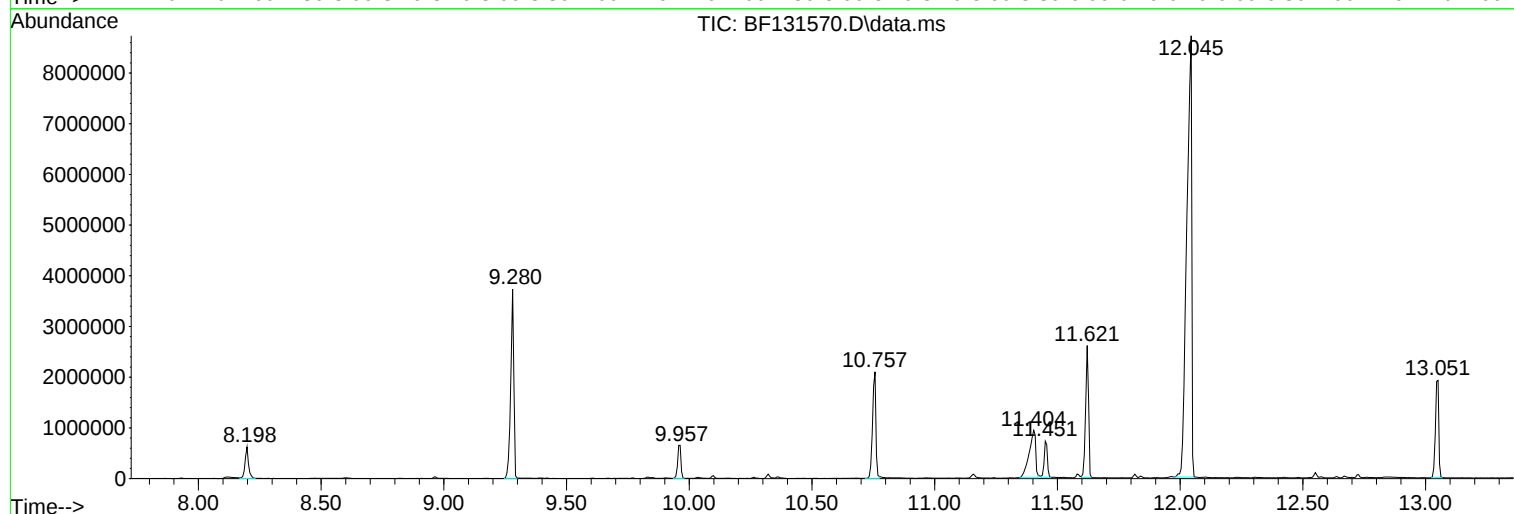
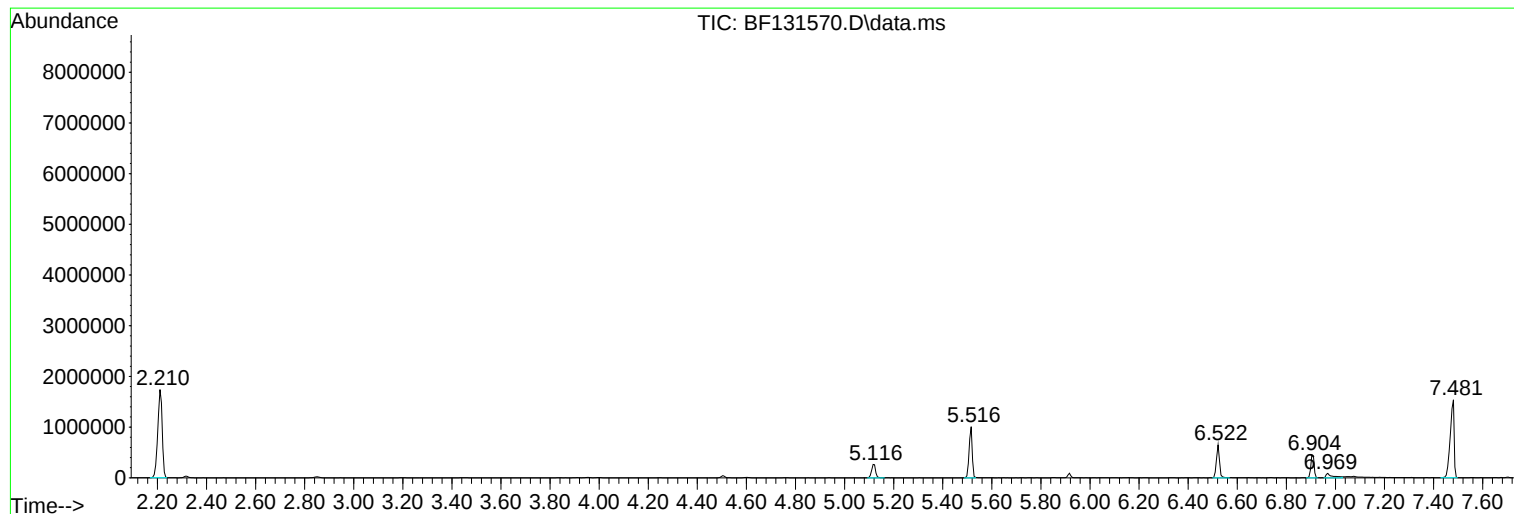
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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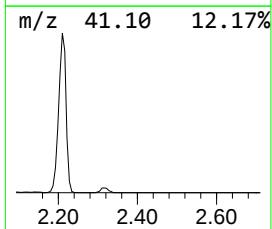
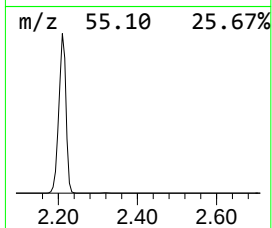
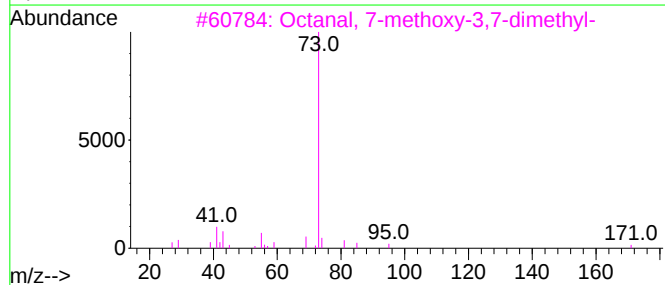
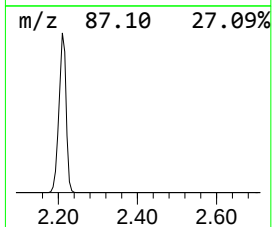
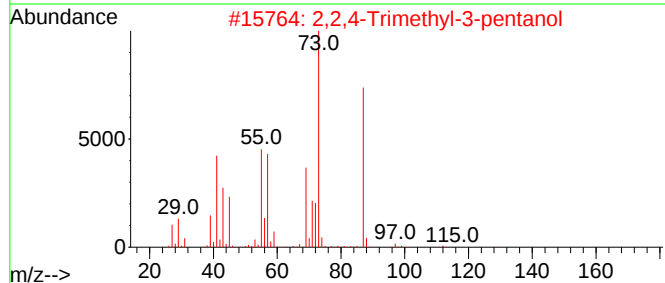
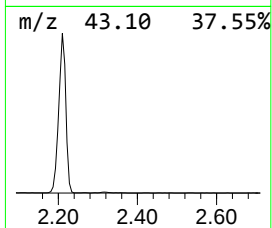
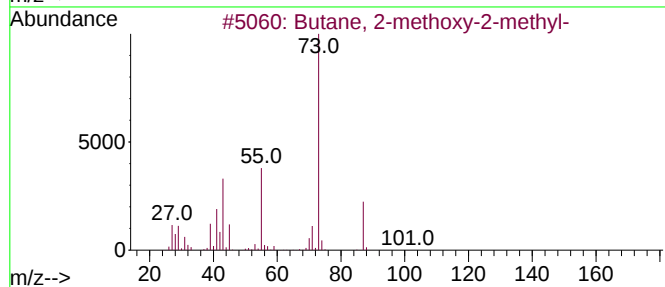
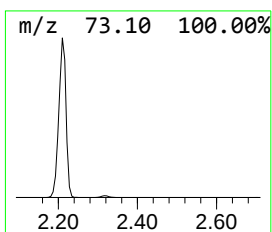
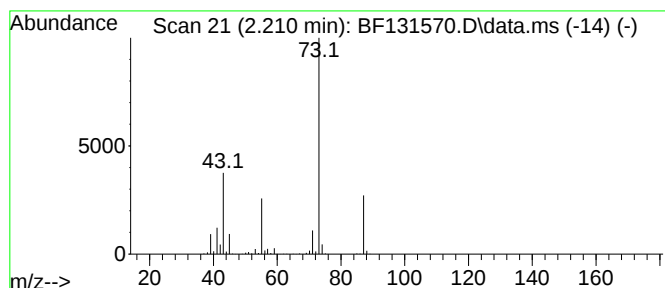
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.210	106.52 ng	2180890	1,4-Dichlorobenzene-d4	6.910

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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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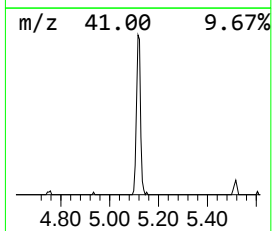
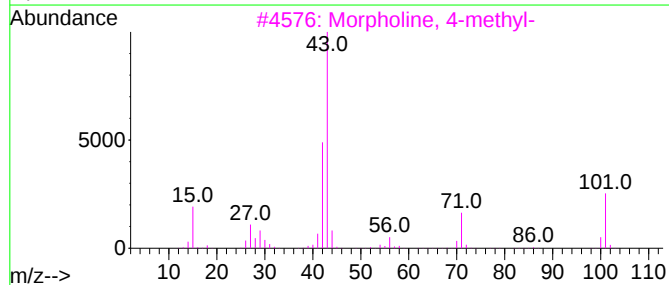
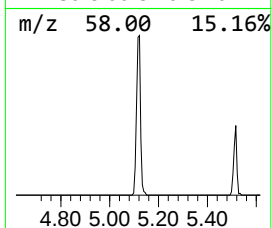
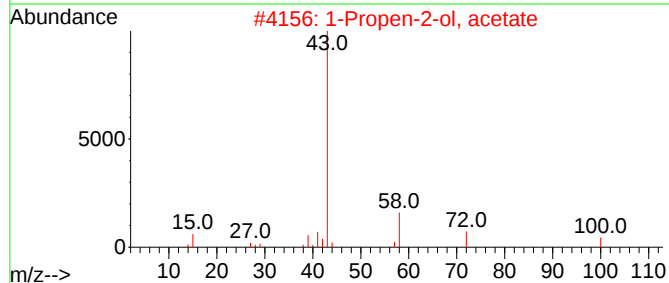
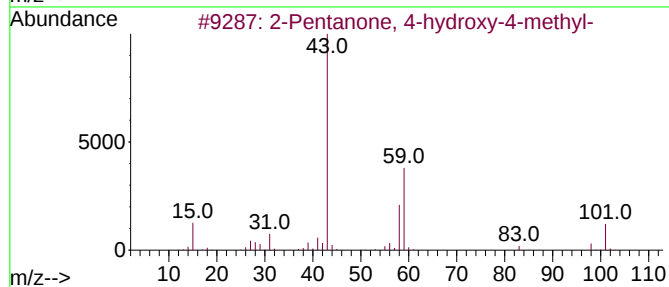
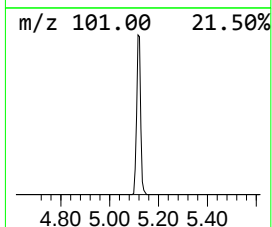
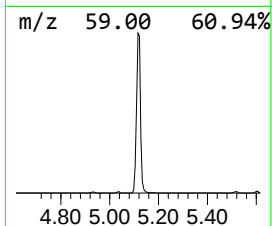
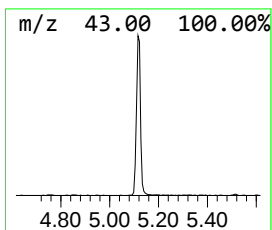
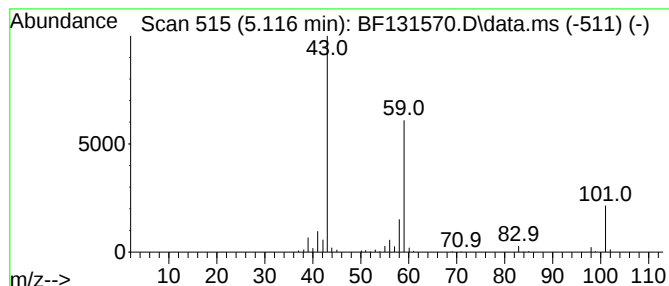
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	14.55 ng	297933	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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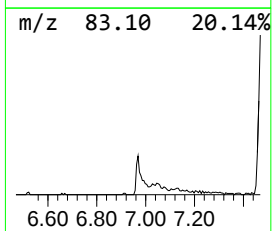
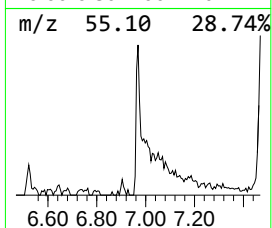
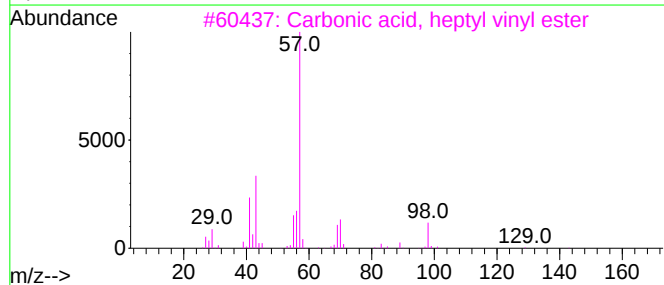
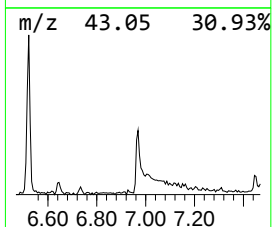
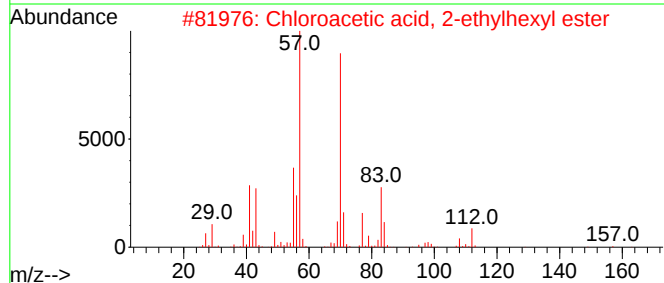
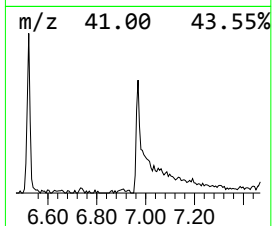
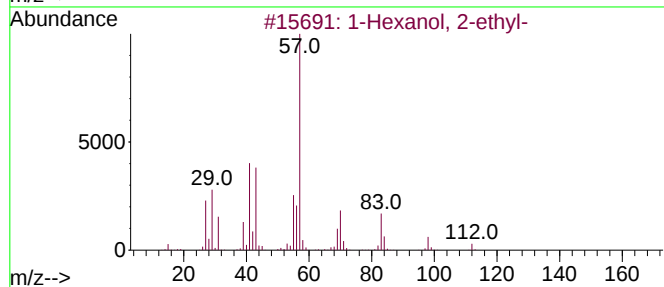
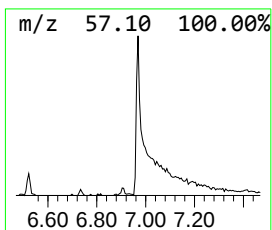
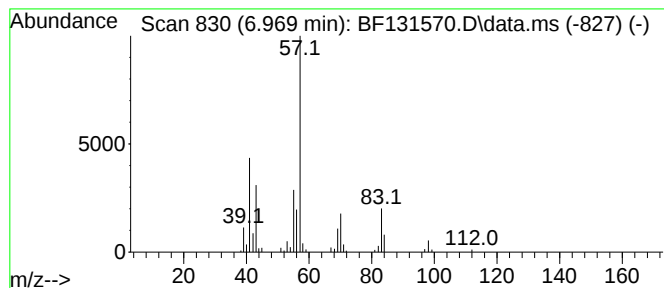
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	7.78 ng	159340	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	72
3			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53
4			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	53
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50



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ALS Vial : 10 Sample Multiplier: 1

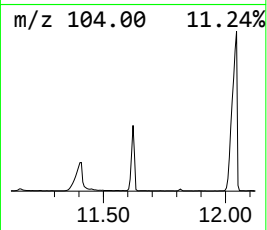
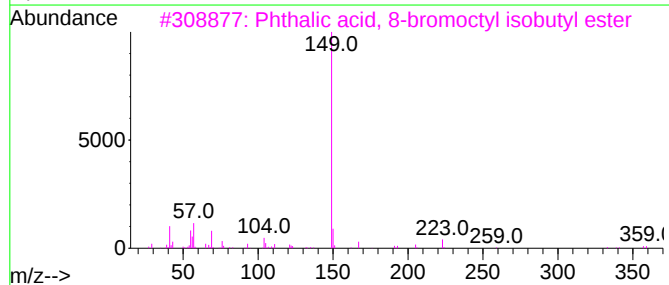
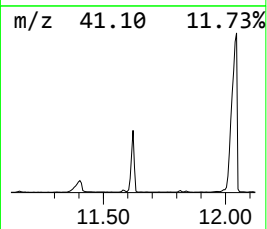
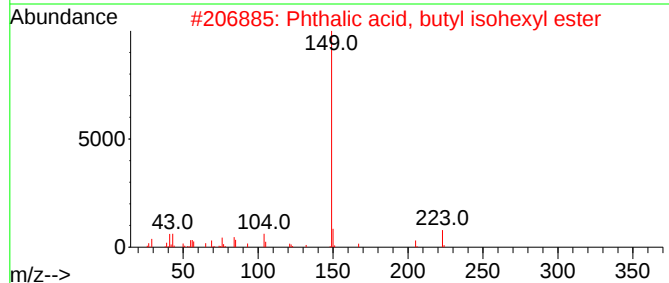
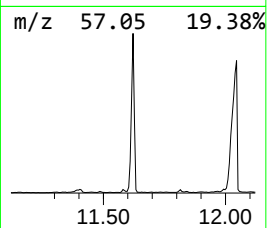
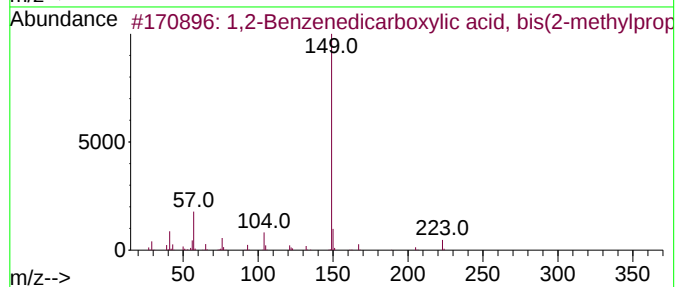
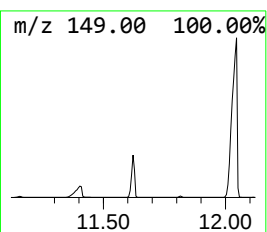
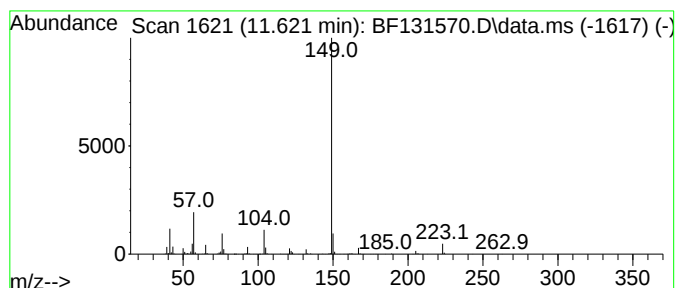
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.621	68.56 ng	2172140	Phenanthrene-d10	11.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2	Phthalic acid, butyl isohexyl ester	306	C18H26O4	1000309-03-6	83
3	Phthalic acid, 8-bromooctyl isobu...	412	C20H29BrO4	1000382-55-3	72
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	72
5	Phthalic acid, cyclohexylmethyl ...	318	C19H26O4	1000309-08-6	72



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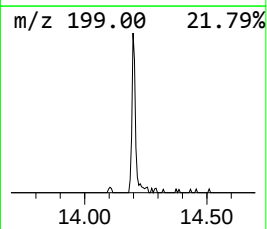
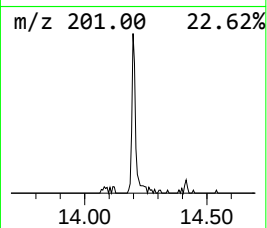
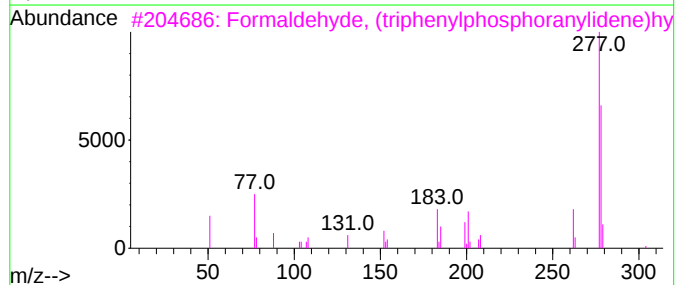
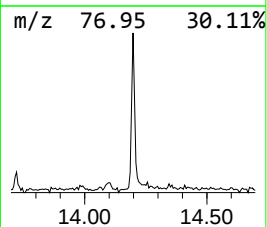
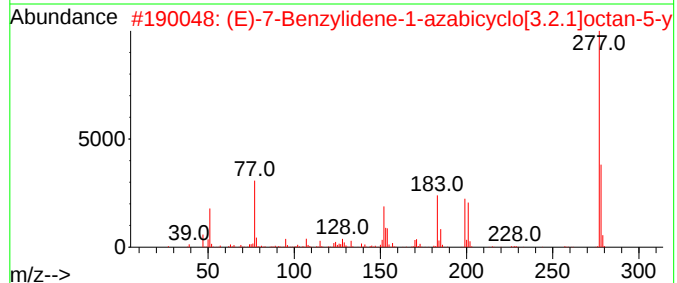
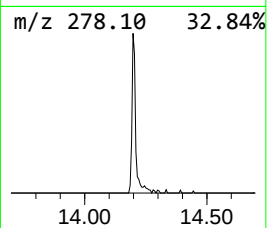
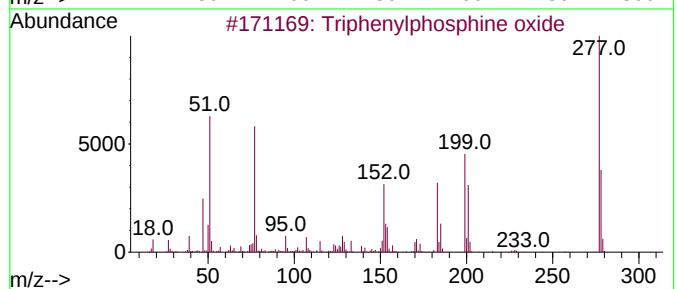
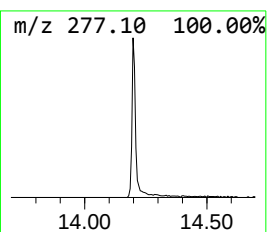
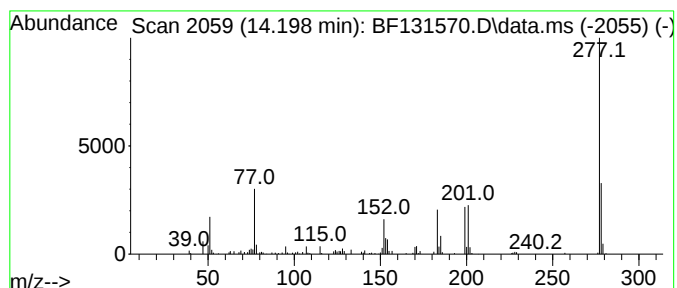
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	5.42 ng	141016	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	38
5			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.210	106.5	ng	2180890	1	6.910	409486	20.0
2-Pentanone, 4-...	5.116	14.6	ng	297933	1	6.910	409486	20.0
1-Hexanol, 2-et...	6.969	7.8	ng	159340	1	6.910	409486	20.0
1,2-Benzenedica...	11.621	68.6	ng	2172140	4	11.451	633618	20.0
Triphenylphosph...	14.198	5.4	ng	141016	5	14.104	520140	20.0