

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071923\
 Data File : BF134356.D
 Acq On : 19 Jul 2023 13:34
 Operator : CG\JU
 Sample : PB154258BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154258BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.493	404	409	413	rBV	1298212	1606678	51.32%	7.139%
2	5.104	505	513	530	rBV	1444484	2387987	76.27%	10.610%
3	5.493	574	579	582	rBV	2683908	2742327	87.59%	12.185%
4	5.863	639	642	647	rBV	61368	54217	1.73%	0.241%
5	6.487	743	748	751	rBV	2136118	2255399	72.04%	10.021%
6	6.840	804	808	823	rVB	550156	460015	14.69%	2.044%
7	7.404	899	904	907	rBV	1437259	1484957	47.43%	6.598%
8	8.116	1021	1025	1029	rBV	761474	588646	18.80%	2.616%
9	9.198	1202	1209	1212	rBV	3358077	2857643	91.27%	12.697%
10	9.875	1320	1324	1328	rBV	868000	684429	21.86%	3.041%
11	10.675	1455	1460	1463	rBV	2334198	2056371	65.68%	9.137%
12	11.369	1574	1578	1582	rBV	827818	744539	23.78%	3.308%
13	12.975	1845	1851	1854	rBV	3247524	3130852	100.00%	13.911%
14	14.033	2027	2031	2039	rBV	702215	628523	20.08%	2.793%
15	14.122	2041	2046	2050	rBV	59541	69699	2.23%	0.310%
16	15.163	2219	2223	2229	rVB	35601	50682	1.62%	0.225%
17	15.539	2282	2287	2294	rBV2	407370	607028	19.39%	2.697%
18	16.010	2364	2367	2372	rVB	34124	51541	1.65%	0.229%
19	16.551	2455	2459	2464	rVB2	27109	44377	1.42%	0.197%

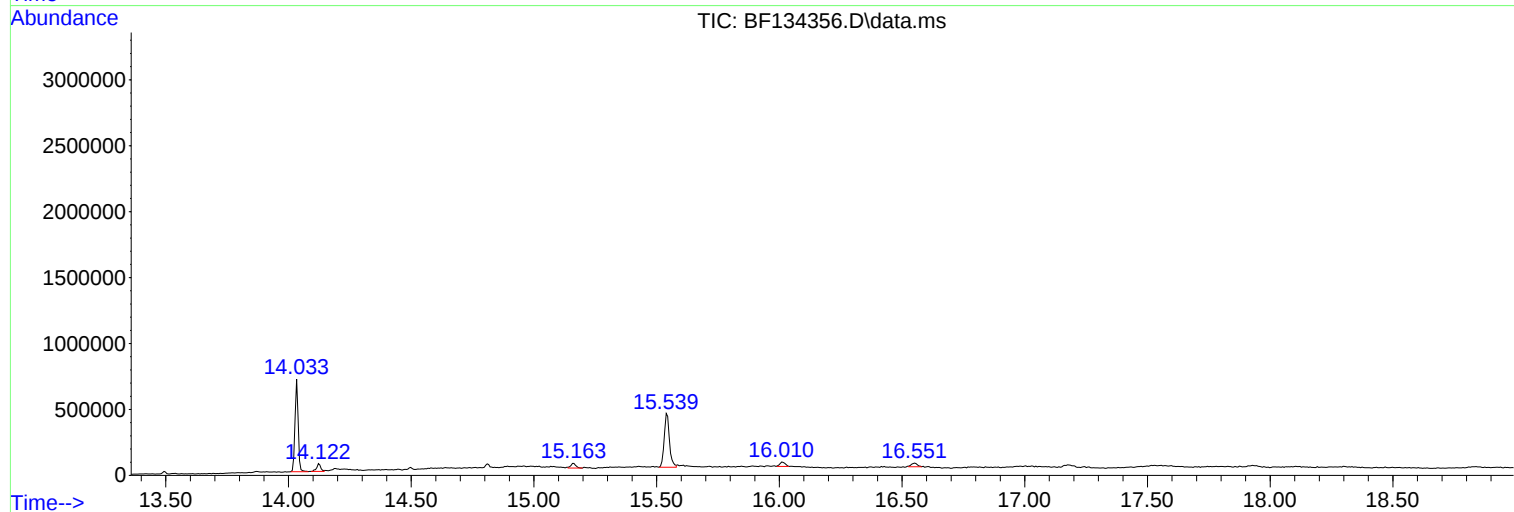
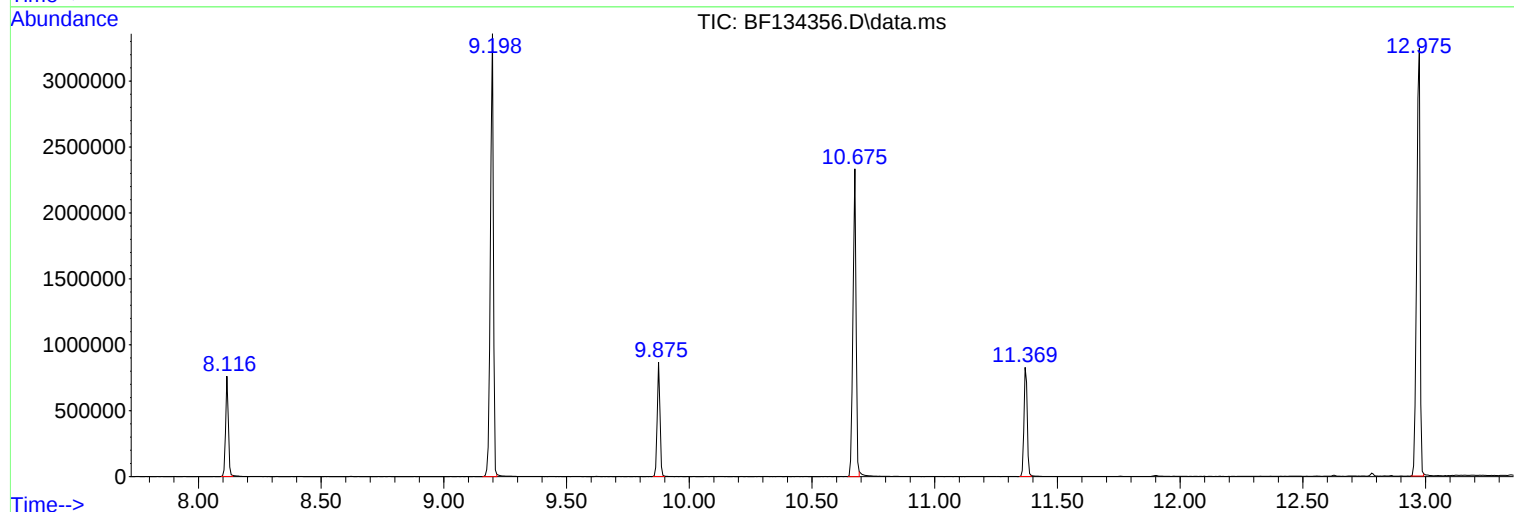
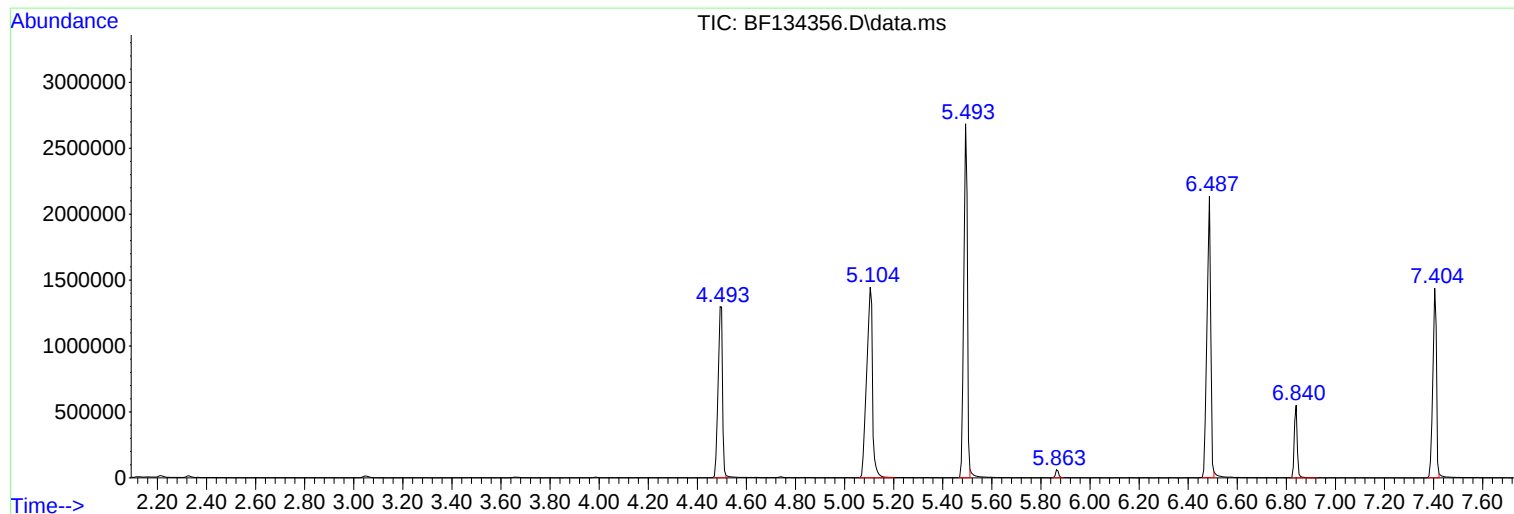
Sum of corrected areas: 22505910

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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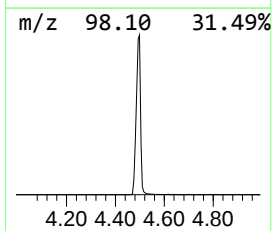
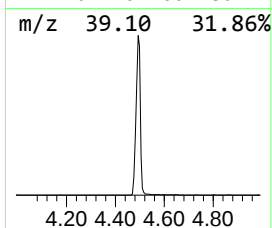
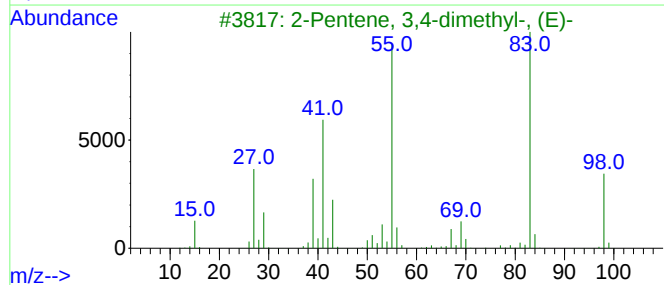
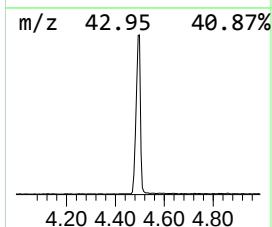
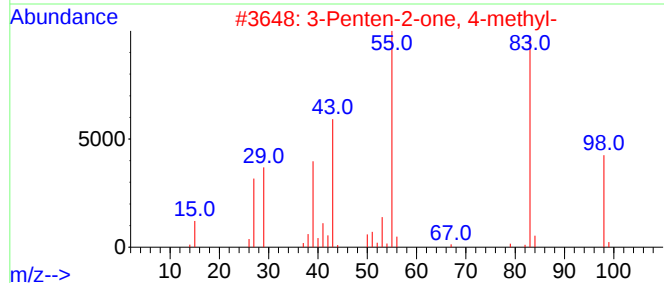
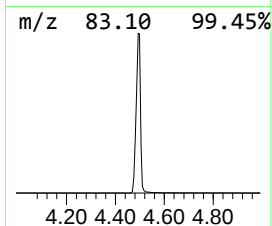
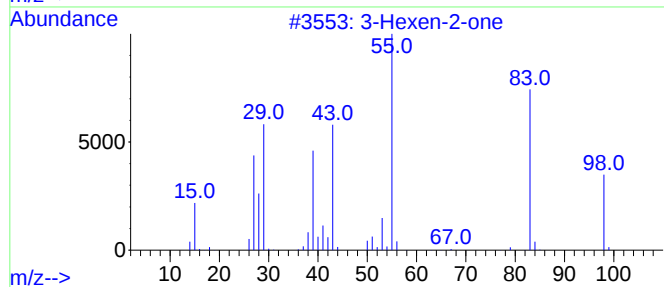
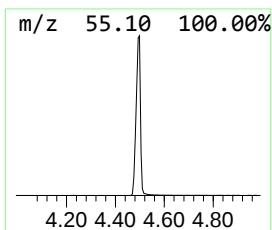
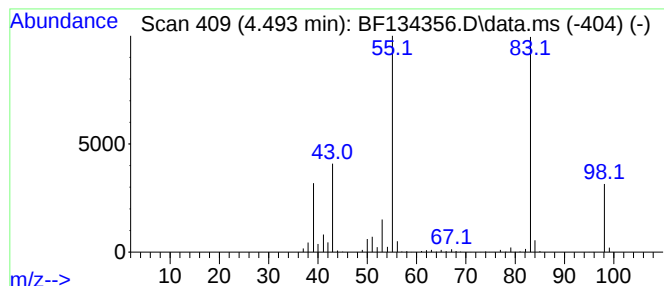
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	69.85 ng	1606680	1,4-Dichlorobenzene-d4	6.840

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one		98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-		98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-		98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-		98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-		98	C7H14	004914-91-4	86



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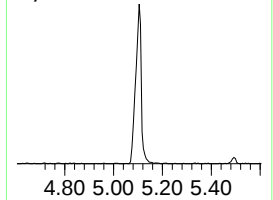
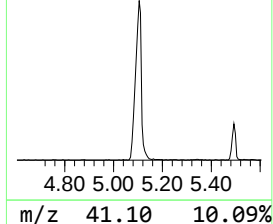
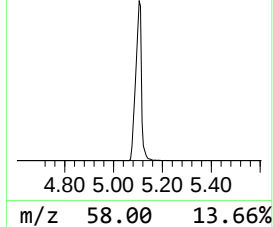
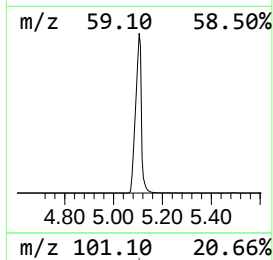
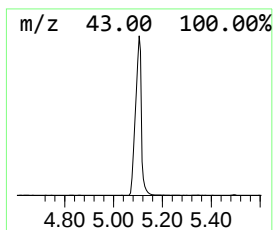
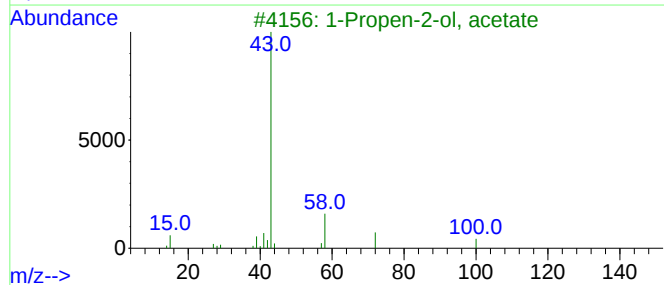
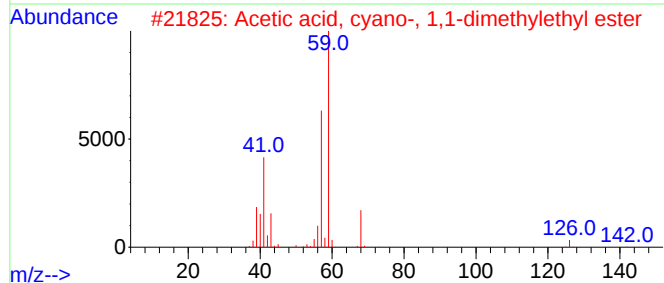
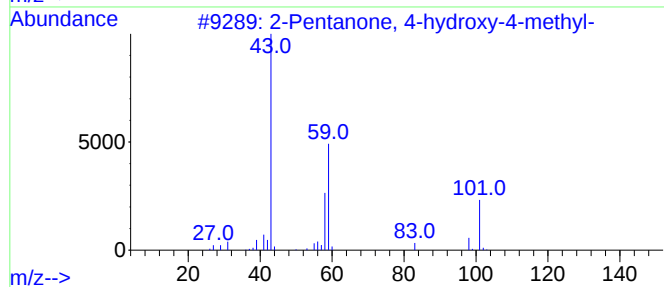
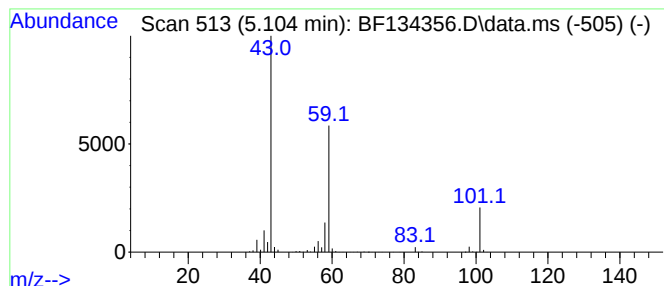
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	103.82 ng	2387990	1,4-Dichlorobenzene-d4	6.840

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9	



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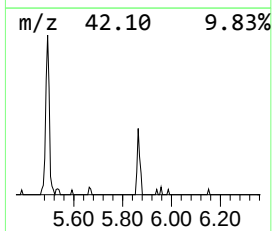
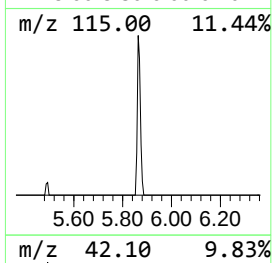
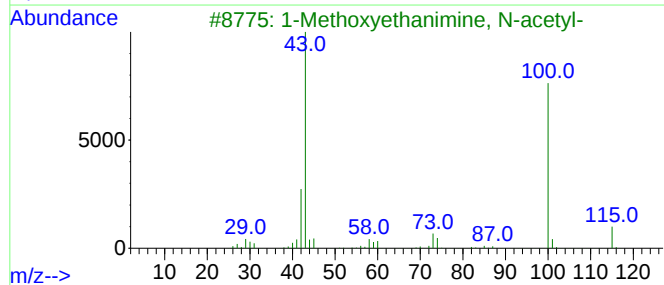
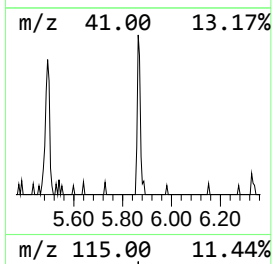
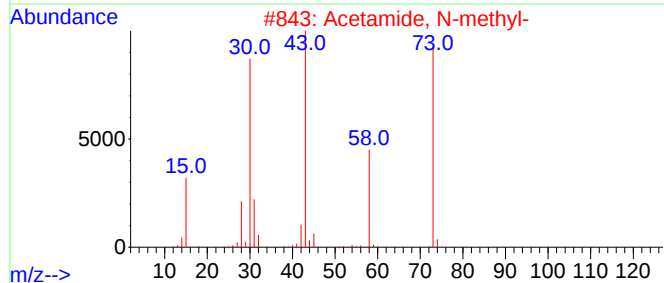
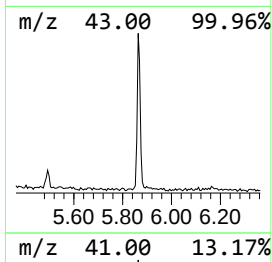
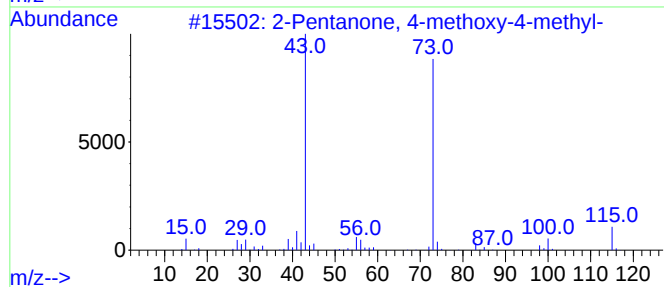
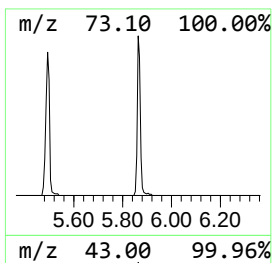
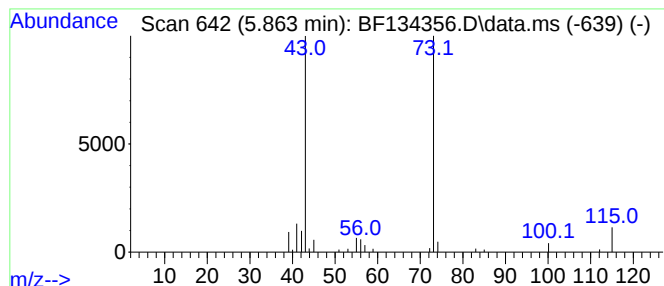
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.863	2.36 ng	54217	1,4-Dichlorobenzene-d4			6.840
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	72
2	Acetamide, N-methyl-		73	C3H7NO	000079-16-3	53
3	1-Methoxyethanimine, N-acetyl-		115	C5H9NO2	099028-43-0	37
4	3-Pentanol, 2,4-dimethyl-		116	C7H16O	000600-36-2	10
5	N-Ethylformamide		73	C3H7NO	000627-45-2	9



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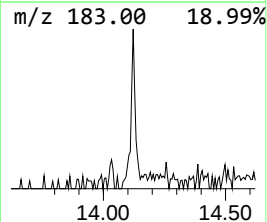
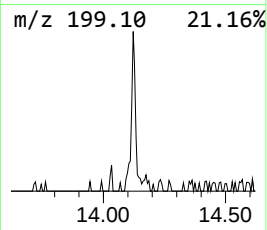
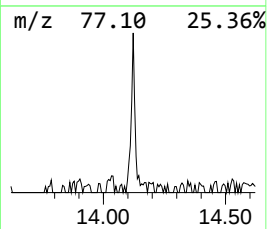
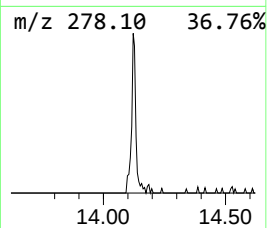
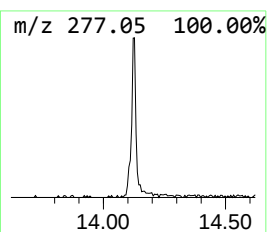
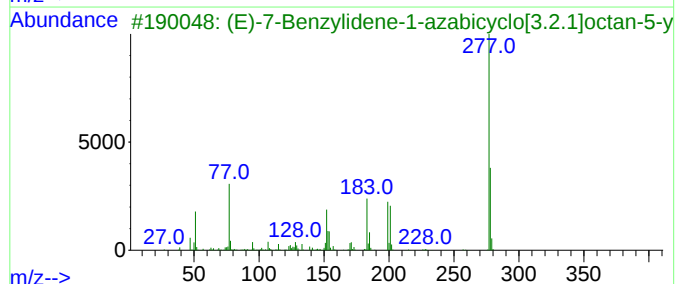
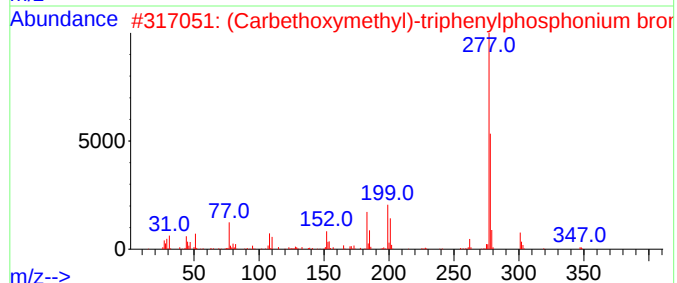
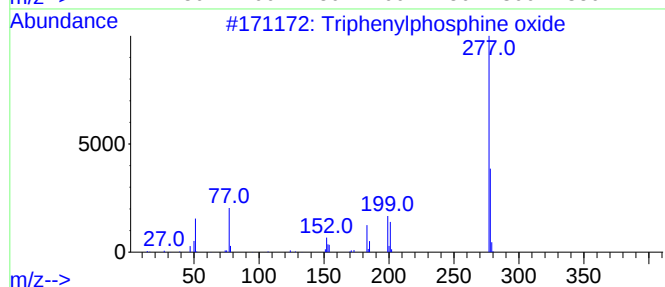
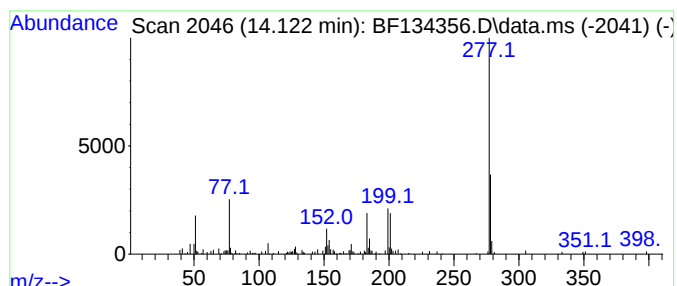
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	2.22 ng	69699	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	50
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.493	69.8	ng	1606680	1	6.840	460015	20.0
2-Pentanone, 4-...	5.104	103.8	ng	2387990	1	6.840	460015	20.0
2-Pentanone, 4-...	5.863	2.4	ng	54217	1	6.840	460015	20.0
Triphenylphosph...	14.121	2.2	ng	69699	5	14.033	628523	20.0