

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122121\
 Data File : BF126293.D
 Acq On : 21 Dec 2021 10:29
 Operator : JU/CG
 Sample : PB141506BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB141506BL

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.410	391	395	404	rBV	274683	306321	6.75%	0.948%
2	5.040	496	502	517	rBV	1517060	2117843	46.65%	6.553%
3	5.440	565	570	573	rBV	4049203	4539767	100.00%	14.046%
4	5.834	634	637	645	rVB	219046	186433	4.11%	0.577%
5	6.445	735	741	744	rBV	3627375	4493751	98.99%	13.904%
6	6.816	800	804	808	rVB	1284243	1013365	22.32%	3.135%
7	7.381	894	900	903	rBV	2959641	3087994	68.02%	9.554%
8	8.098	1017	1022	1034	rBV	1492523	1412765	31.12%	4.371%
9	9.180	1200	1206	1209	rBV	4033936	4383745	96.56%	13.563%
10	9.851	1316	1320	1333	rBV	1363903	1443483	31.80%	4.466%
11	10.639	1450	1454	1472	rBV	2321183	2634747	58.04%	8.152%
12	11.339	1569	1573	1580	rBV	1428629	1328654	29.27%	4.111%
13	12.927	1838	1843	1846	rBV	3485092	3627319	79.90%	11.223%
14	13.974	2017	2021	2032	rBV	768531	807097	17.78%	2.497%
15	14.068	2032	2037	2046	rVV	164671	204183	4.50%	0.632%
16	15.421	2262	2267	2273	rBV	504762	733460	16.16%	2.269%

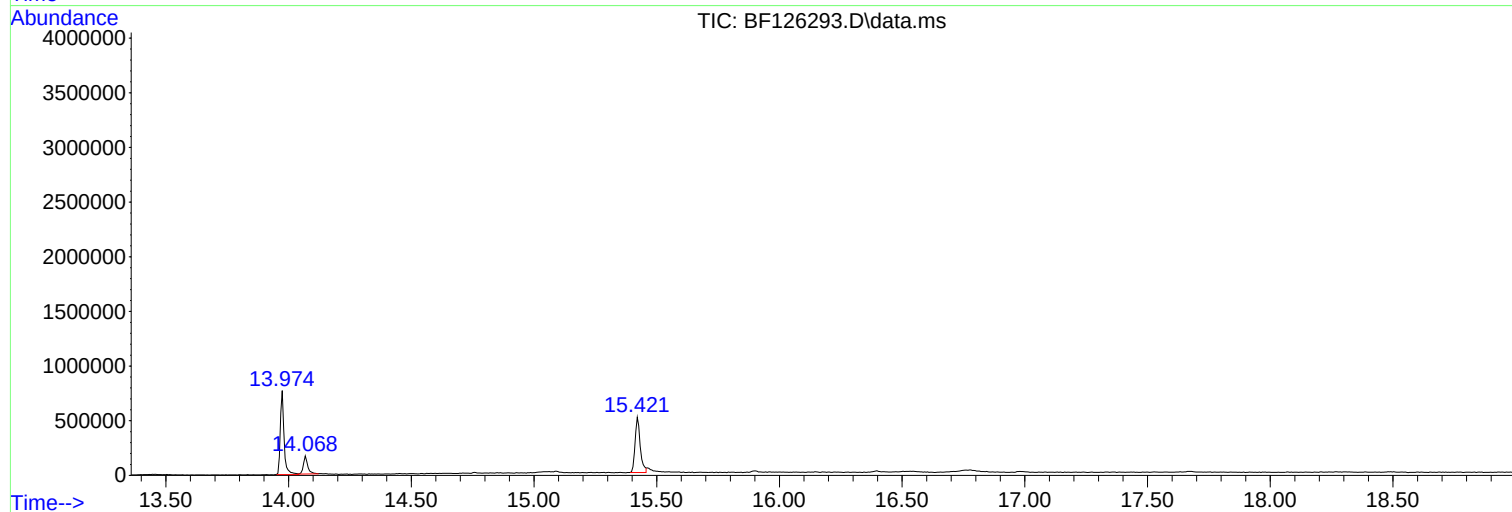
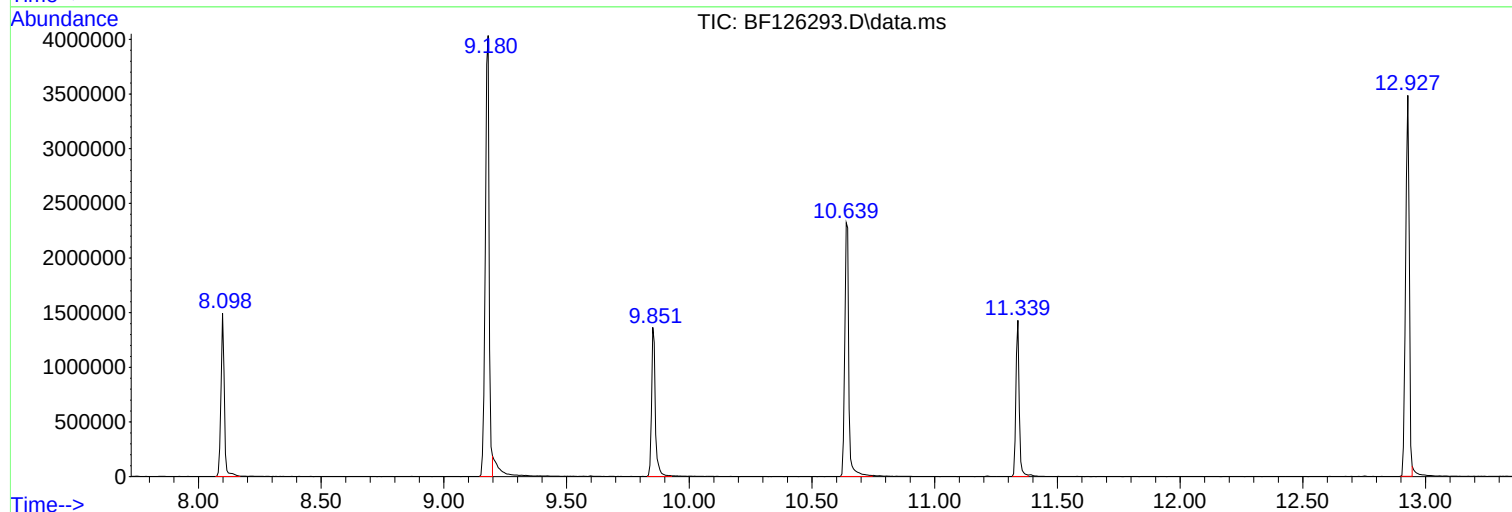
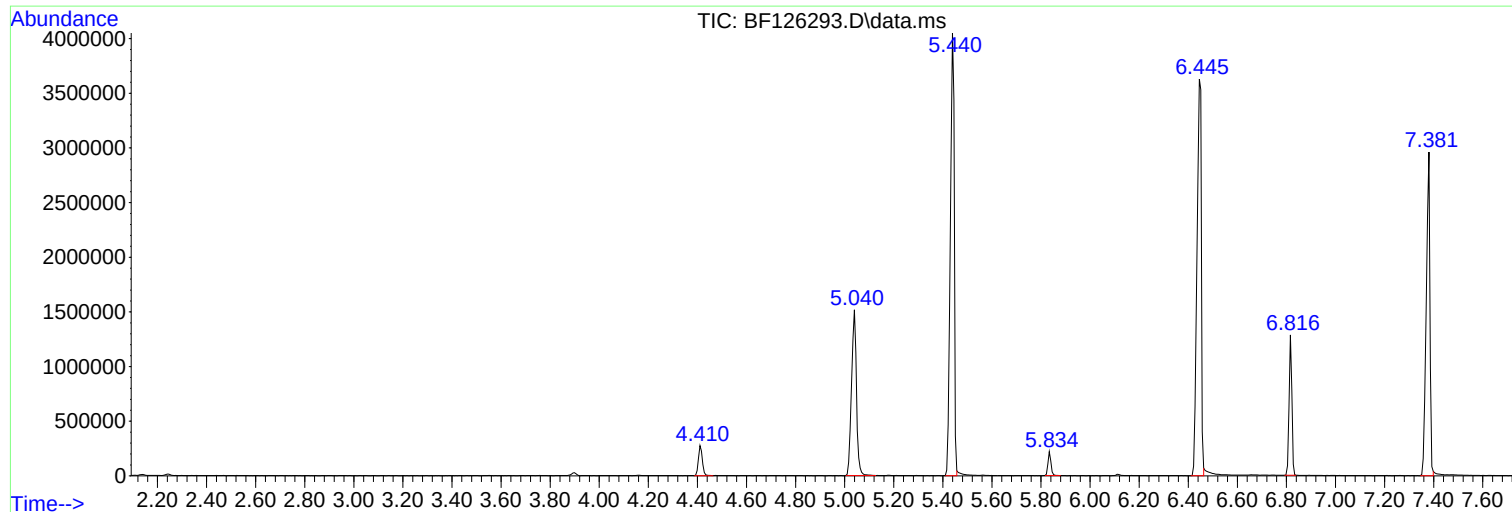
Sum of corrected areas: 32320927

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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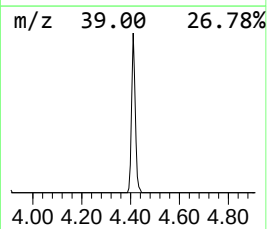
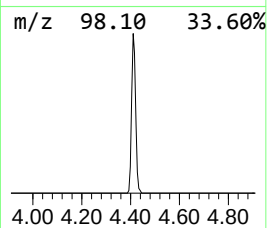
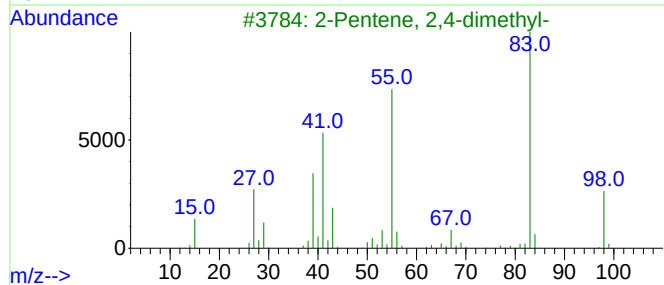
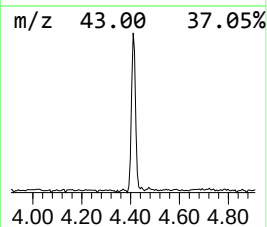
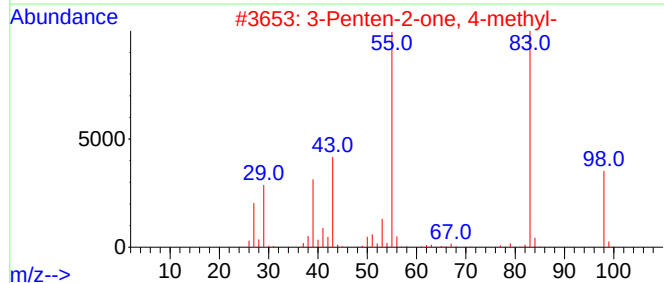
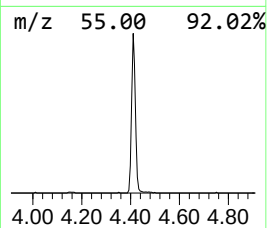
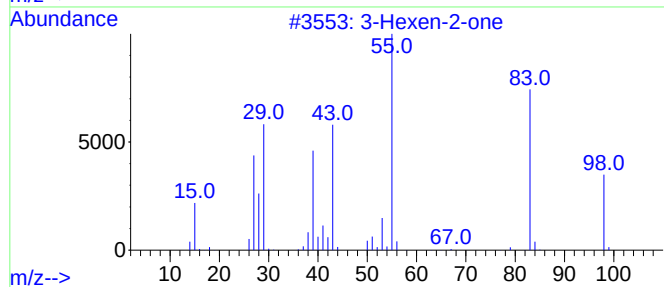
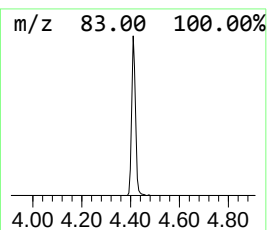
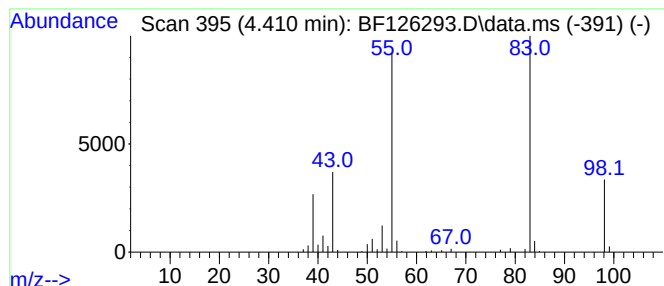
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.410	6.05 ng	306321	1,4-Dichlorobenzene-d4	6.816

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, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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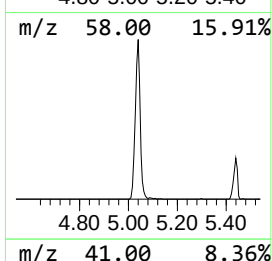
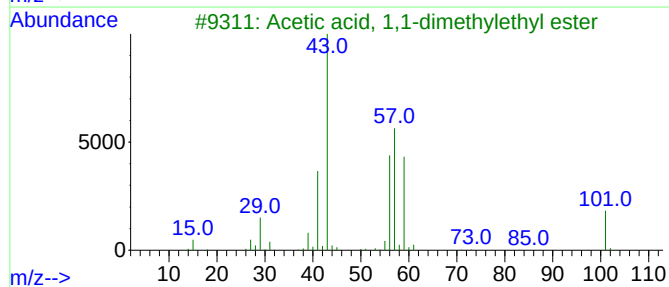
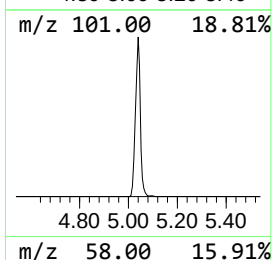
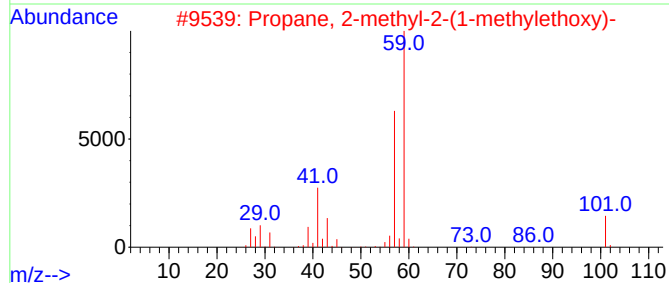
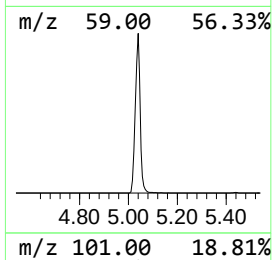
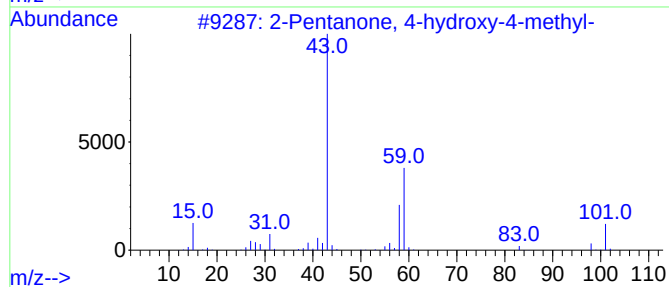
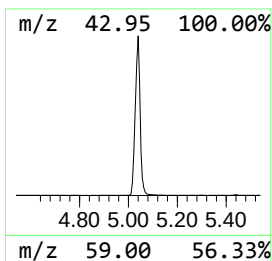
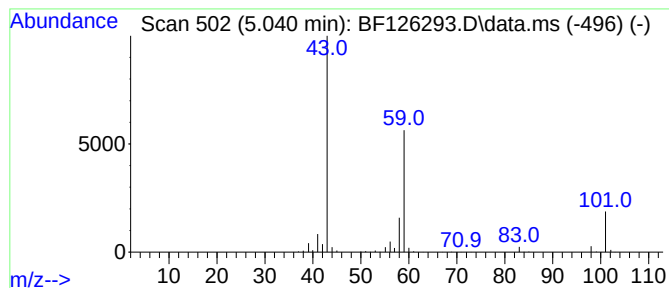
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	41.80 ng	2117840	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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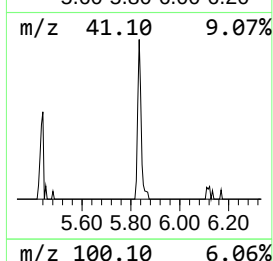
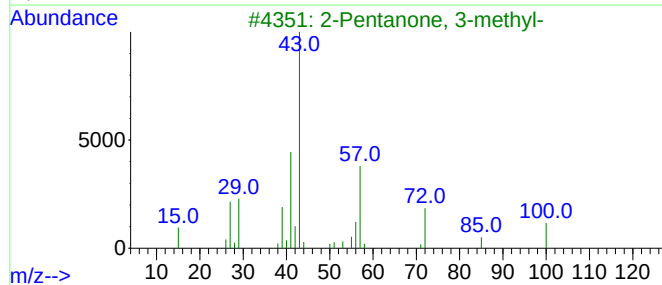
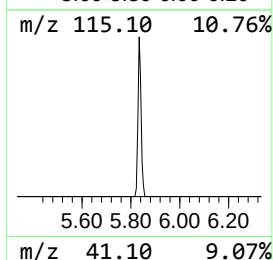
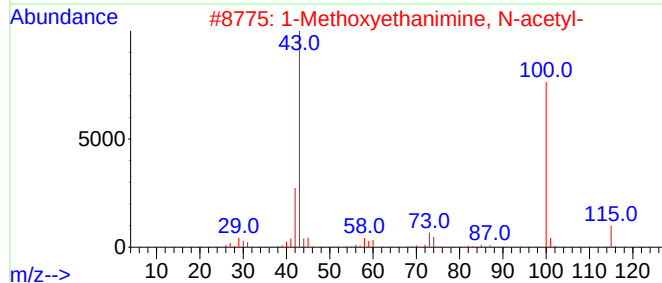
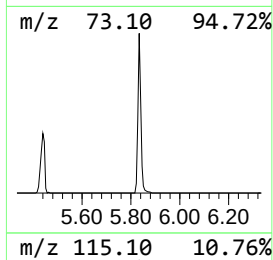
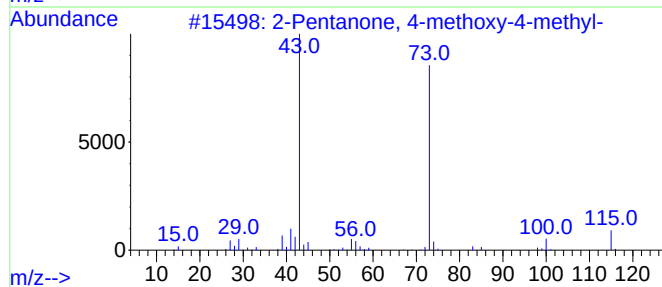
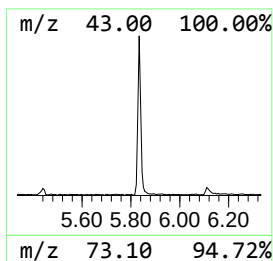
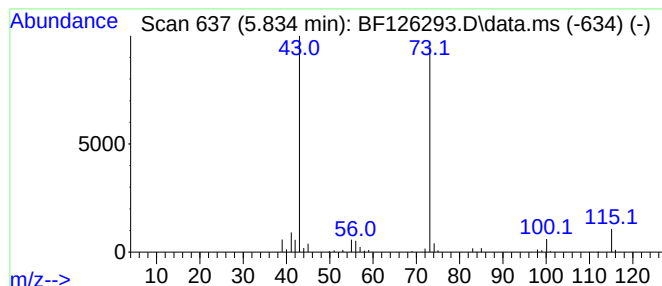
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	3.68 ng	186433	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
3			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
4			Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5			N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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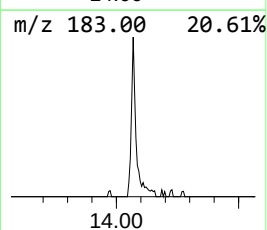
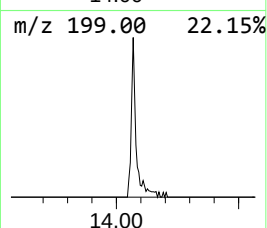
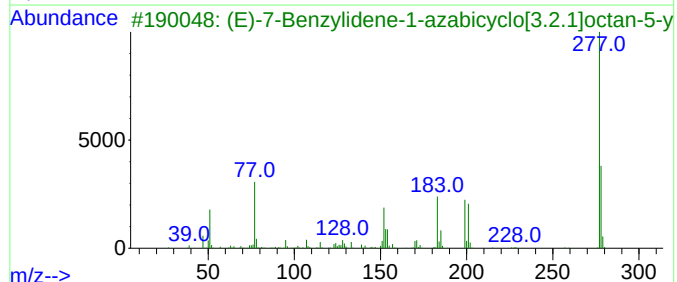
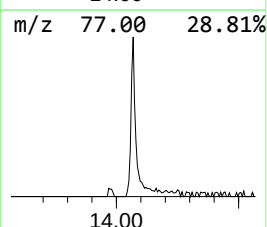
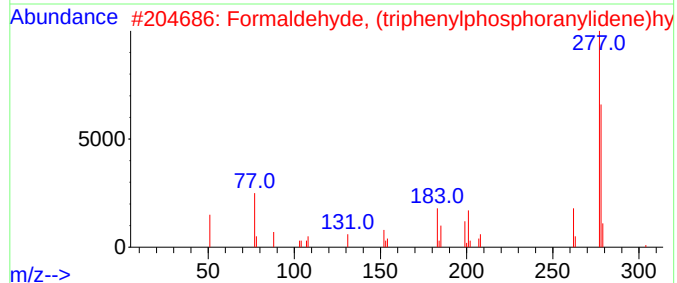
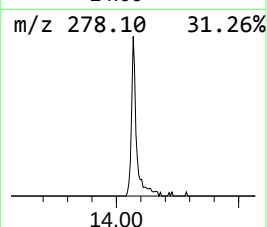
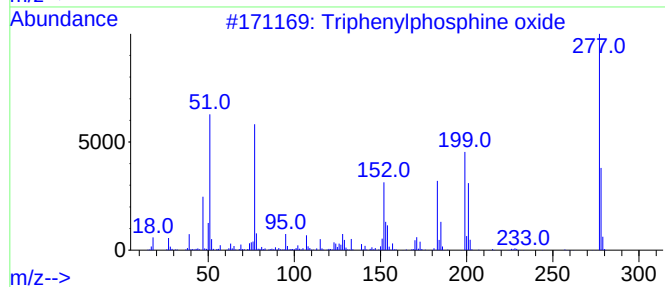
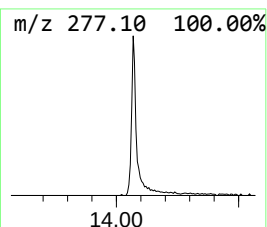
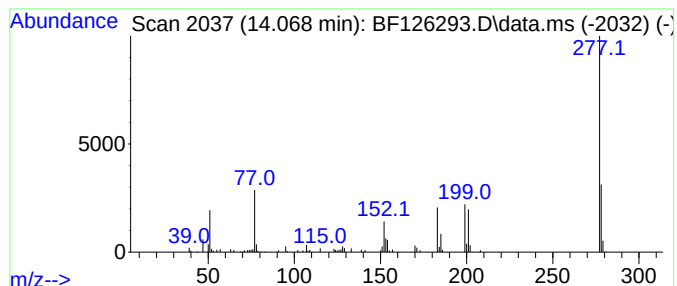
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	5.06 ng	204183	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	46
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2N0S2	017046-34-3	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.410	6.0	ng	306321	1	6.816	1013370	20.0
2-Pentanone, 4-...	5.040	41.8	ng	2117840	1	6.816	1013370	20.0
2-Pentanone, 4-...	5.834	3.7	ng	186433	1	6.816	1013370	20.0
Triphenylphosph...	14.068	5.1	ng	204183	5	13.974	807097	20.0