

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
 Data File : BF130838.D
 Acq On : 28 Oct 2022 22:59
 Operator : CG\JU
 Sample : N5281-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5S

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: BF130838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	30	39	48	rVB	1555313	2042584	73.81%	9.431%
2	3.528	242	245	261	rBV	23302	44131	1.59%	0.204%
3	5.181	522	526	535	rVB	378028	467293	16.89%	2.157%
4	5.563	586	591	594	rBV	2283409	2378131	85.94%	10.980%
5	6.557	754	760	763	rBV	2276279	2470178	89.27%	11.405%
6	6.945	822	826	829	rBV	822144	677632	24.49%	3.129%
7	7.504	916	921	924	rBV	1551962	1544850	55.83%	7.133%
8	8.228	1039	1044	1048	rBV	962557	893343	32.28%	4.125%
9	9.304	1222	1227	1231	rBV	2677743	2767172	100.00%	12.776%
10	9.986	1338	1343	1347	rBV	1072168	1012067	36.57%	4.673%
11	10.781	1471	1478	1481	rBV	1917616	1721727	62.22%	7.949%
12	11.480	1593	1597	1600	rBV	1298356	1029191	37.19%	4.752%
13	11.545	1604	1608	1611	rVB2	48317	35162	1.27%	0.162%
14	11.998	1679	1685	1689	rBV	40006	40427	1.46%	0.187%
15	13.075	1863	1868	1871	rVB	2656171	2613984	94.46%	12.069%
16	13.986	2018	2023	2037	rBV2	117798	304687	11.01%	1.407%
17	14.127	2043	2047	2050	rVB	870992	787146	28.45%	3.634%
18	14.221	2058	2063	2070	rBV	205415	221219	7.99%	1.021%
19	15.639	2298	2304	2309	rBV	471436	578280	20.90%	2.670%
20	16.268	2403	2411	2414	rBV7	10876	30032	1.09%	0.139%

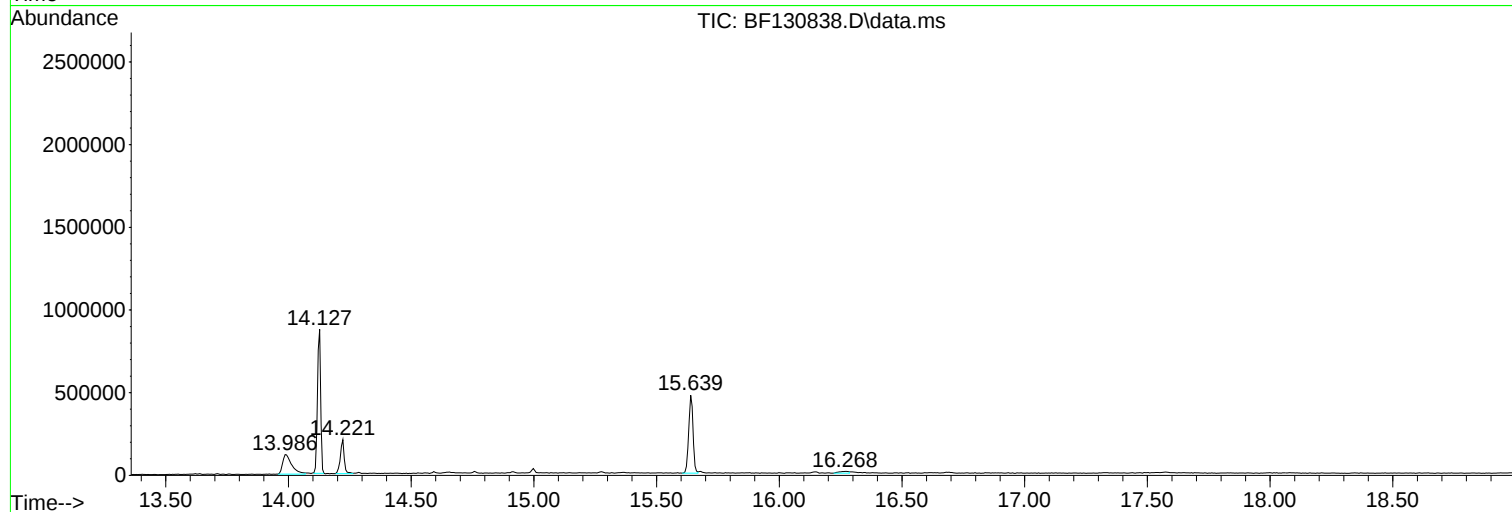
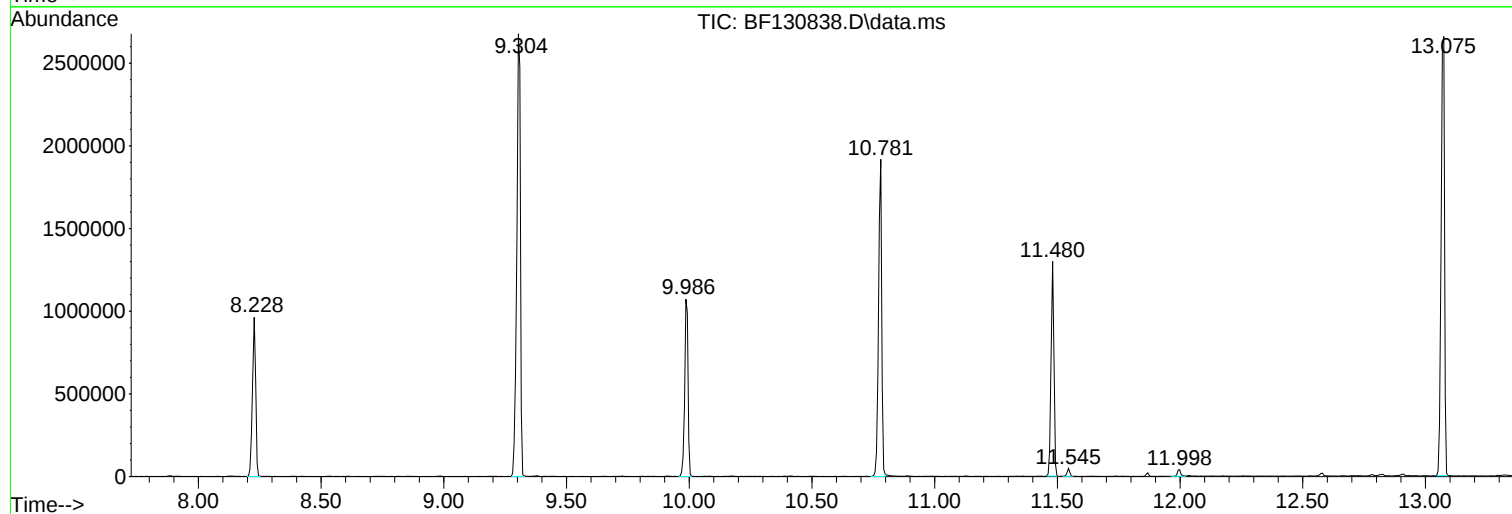
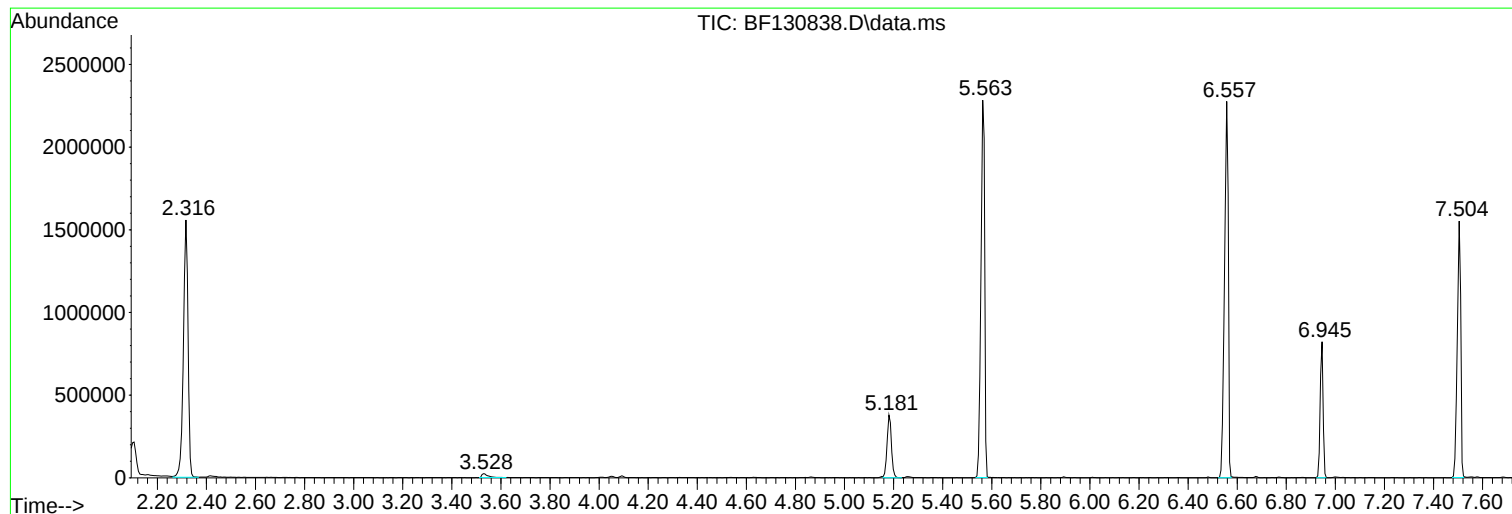
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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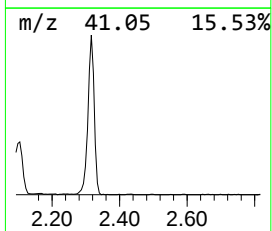
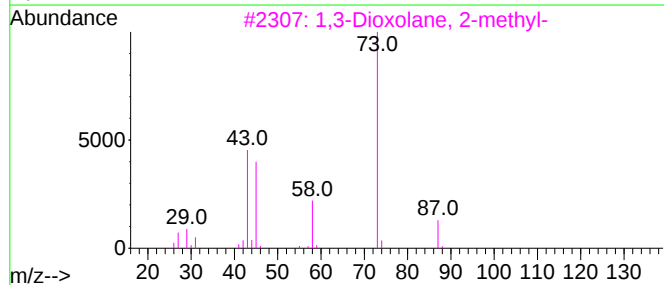
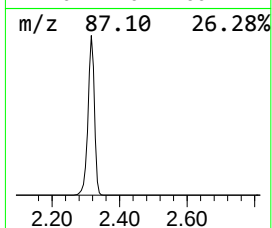
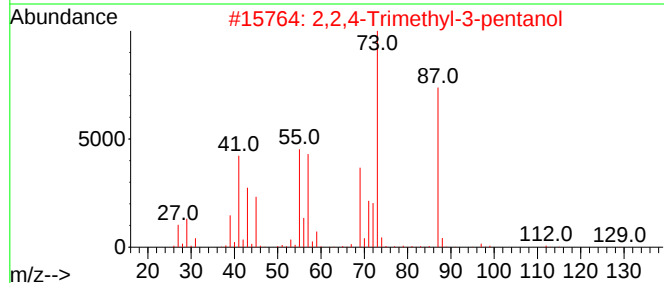
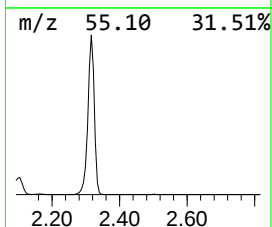
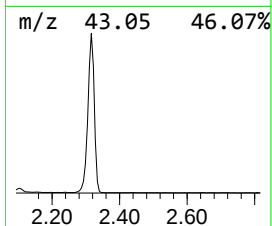
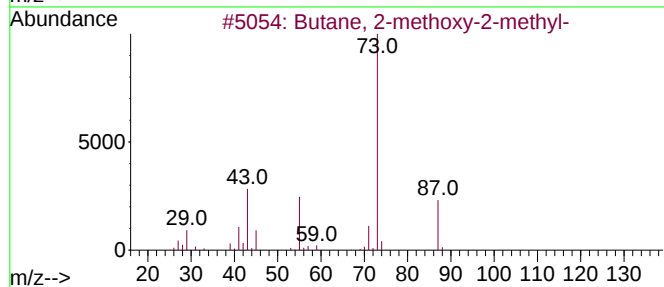
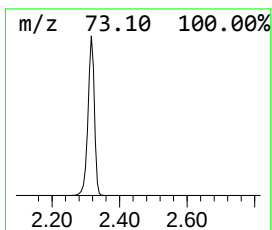
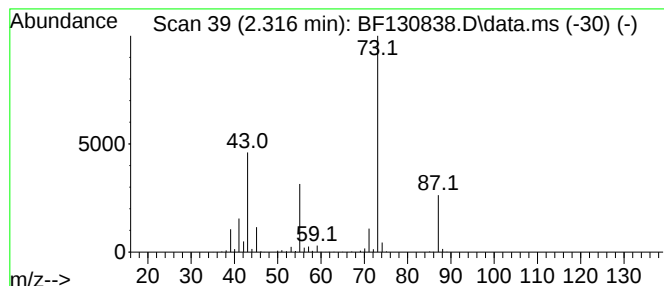
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.316	60.29 ng	2042580	1,4-Dichlorobenzene-d4	6.945

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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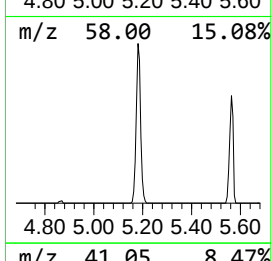
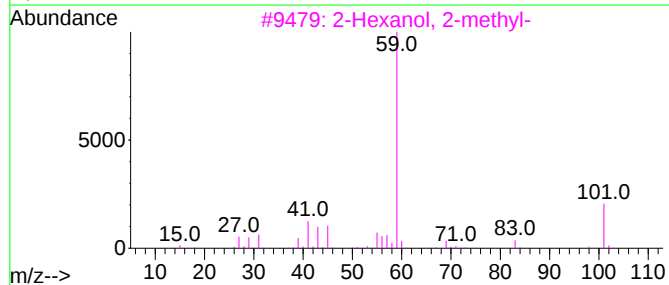
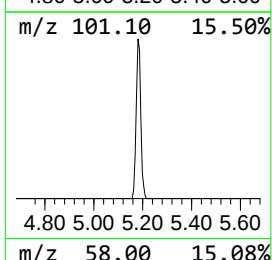
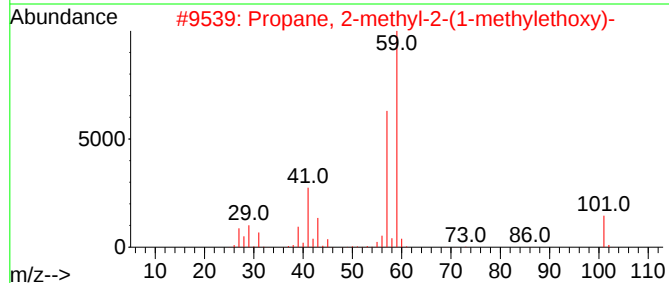
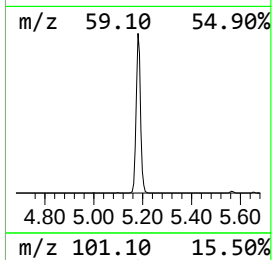
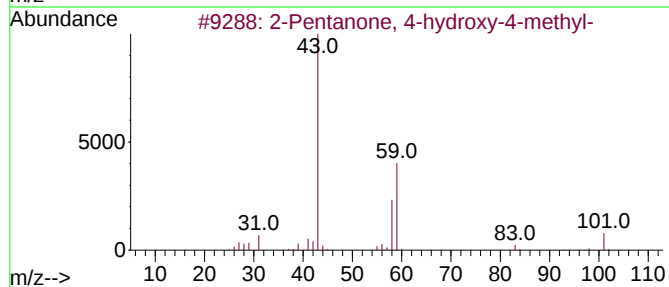
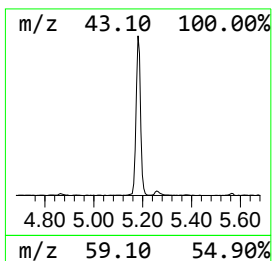
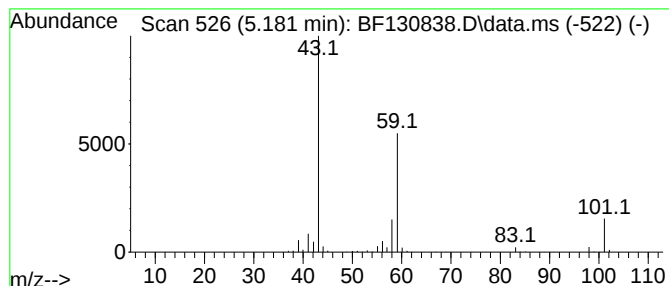
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	13.79 ng	467293	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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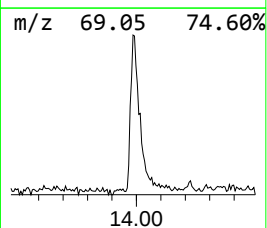
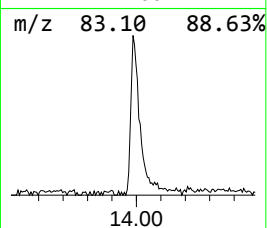
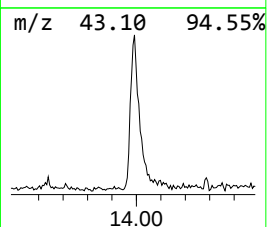
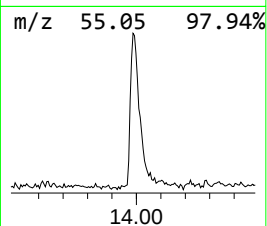
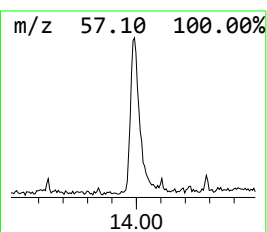
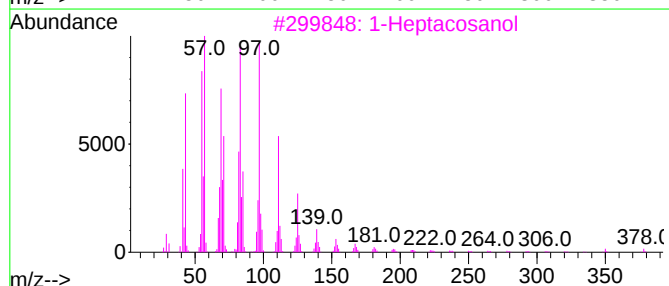
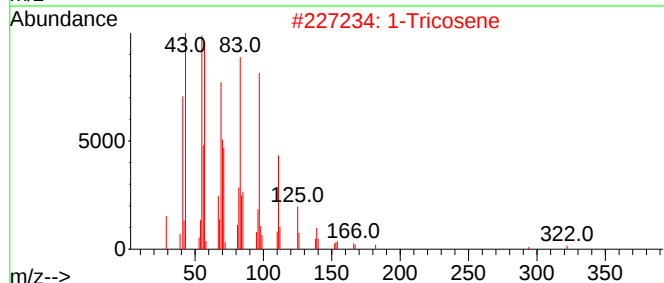
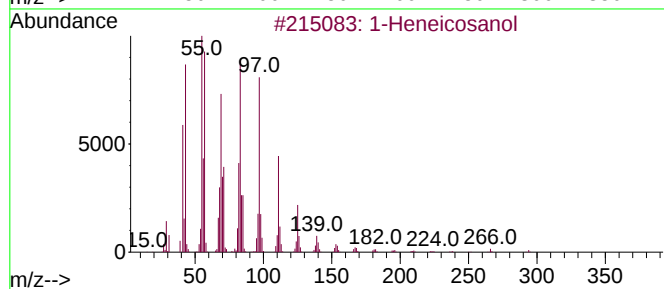
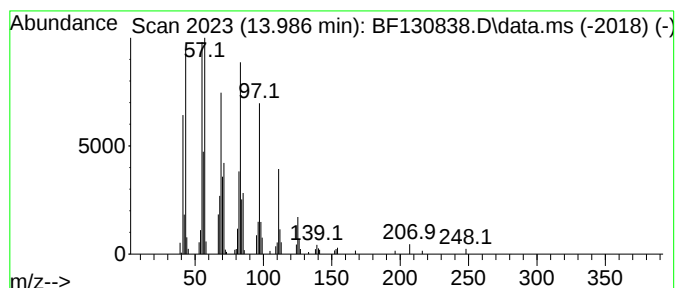
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	7.74 ng	304687	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			1-Tricosene	322	C23H46	018835-32-0	93
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



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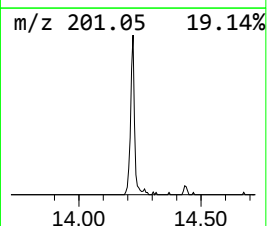
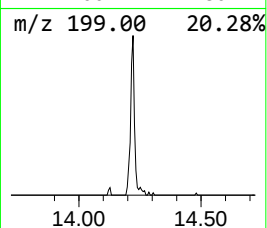
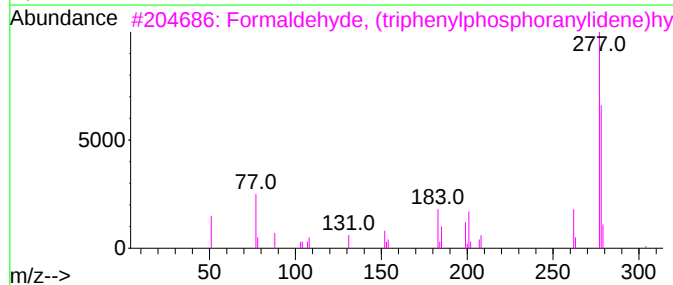
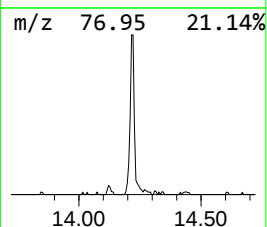
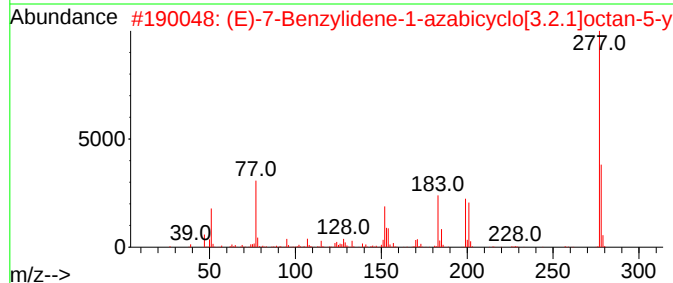
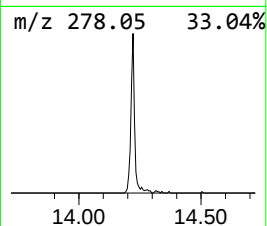
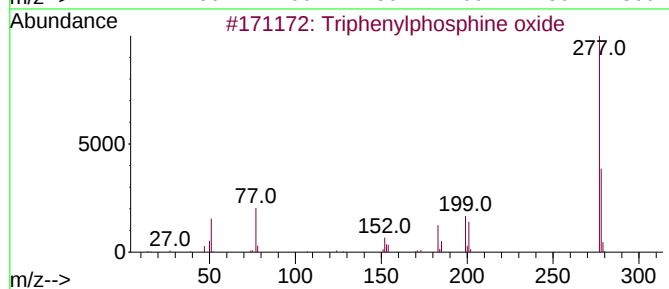
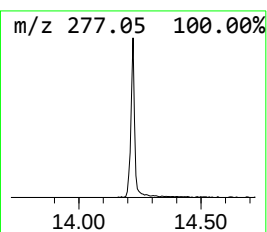
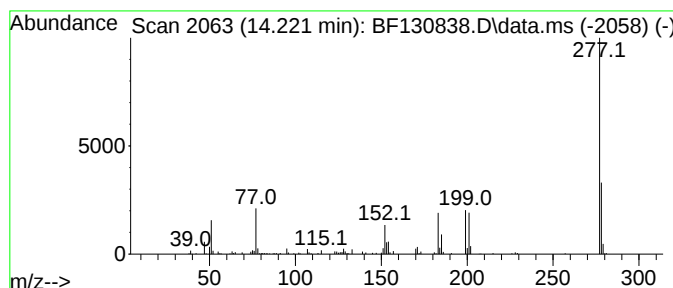
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.222	5.62 ng	221219	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	37
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	17



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.316	60.3	ng	2042580	1	6.945	677632	20.0
2-Pentanone, 4-...	5.181	13.8	ng	467293	1	6.945	677632	20.0
1-Heneicosanol	13.986	7.7	ng	304687	5	14.127	787146	20.0
Triphenylphosph...	14.222	5.6	ng	221219	5	14.127	787146	20.0