

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
 Data File : BF131405.D
 Acq On : 25 Nov 2022 20:19
 Operator : CG\JU
 Sample : N5741-17
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-36

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	22	29	36	rVB	1621619	2067875	67.50%	10.912%
2	5.175	520	525	530	rVB	192412	222675	7.27%	1.175%
3	5.563	586	591	594	rBV	1590450	1443984	47.13%	7.620%
4	6.563	756	761	764	rBV	1070970	950343	31.02%	5.015%
5	6.951	824	827	831	rVB	645390	573376	18.72%	3.026%
6	7.522	918	924	927	rBV	1799866	1806863	58.98%	9.534%
7	8.245	1042	1047	1050	rBV	845594	735702	24.01%	3.882%
8	9.328	1225	1231	1234	rBV	3457190	3063689	100.00%	16.167%
9	10.010	1340	1347	1350	rBV	1059355	856795	27.97%	4.521%
10	10.728	1465	1469	1474	rVB	181053	142303	4.64%	0.751%
11	10.804	1477	1482	1485	rBV	2384712	2100576	68.56%	11.084%
12	11.504	1597	1601	1605	rBV	1012445	863013	28.17%	4.554%
13	12.280	1731	1733	1742	rVB2	44368	45020	1.47%	0.238%
14	13.104	1868	1873	1876	rBV	2877934	2607984	85.13%	13.762%
15	13.998	2022	2025	2038	rBV	158168	227183	7.42%	1.199%
16	14.163	2049	2053	2057	rVB	659626	569442	18.59%	3.005%
17	14.263	2065	2070	2076	rBV	88517	91717	2.99%	0.484%
18	15.698	2309	2314	2319	rBV	369401	503491	16.43%	2.657%
19	16.204	2396	2400	2408	rBV	26312	36391	1.19%	0.192%
20	16.757	2490	2494	2500	rVB3	23837	42374	1.38%	0.224%

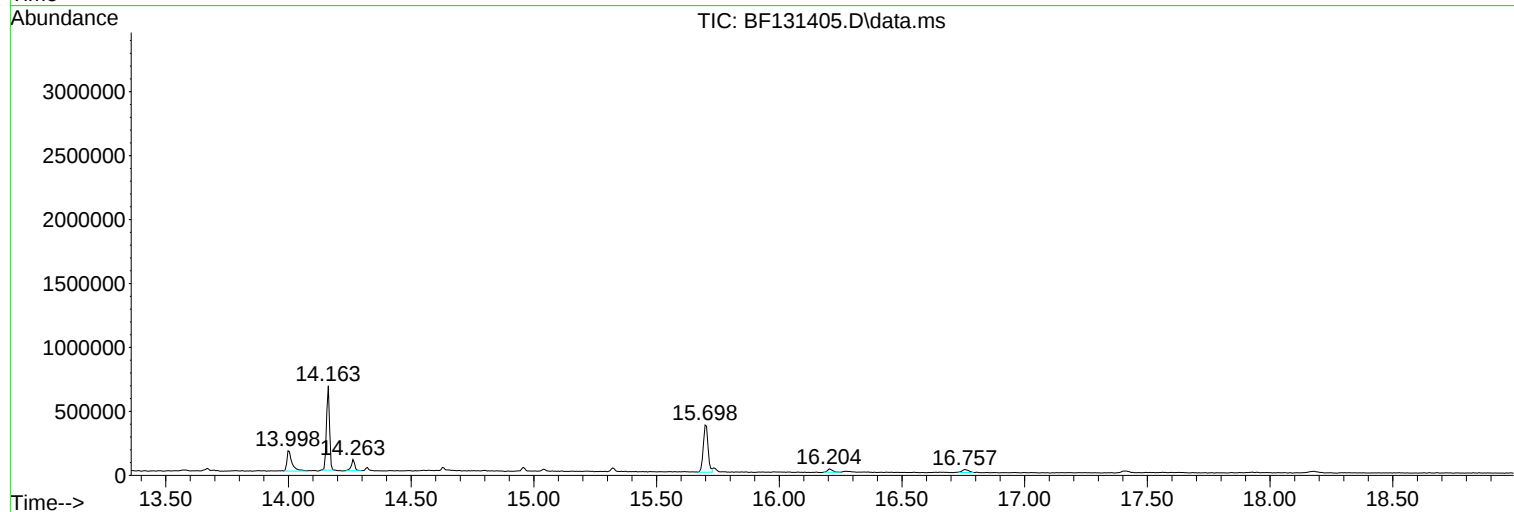
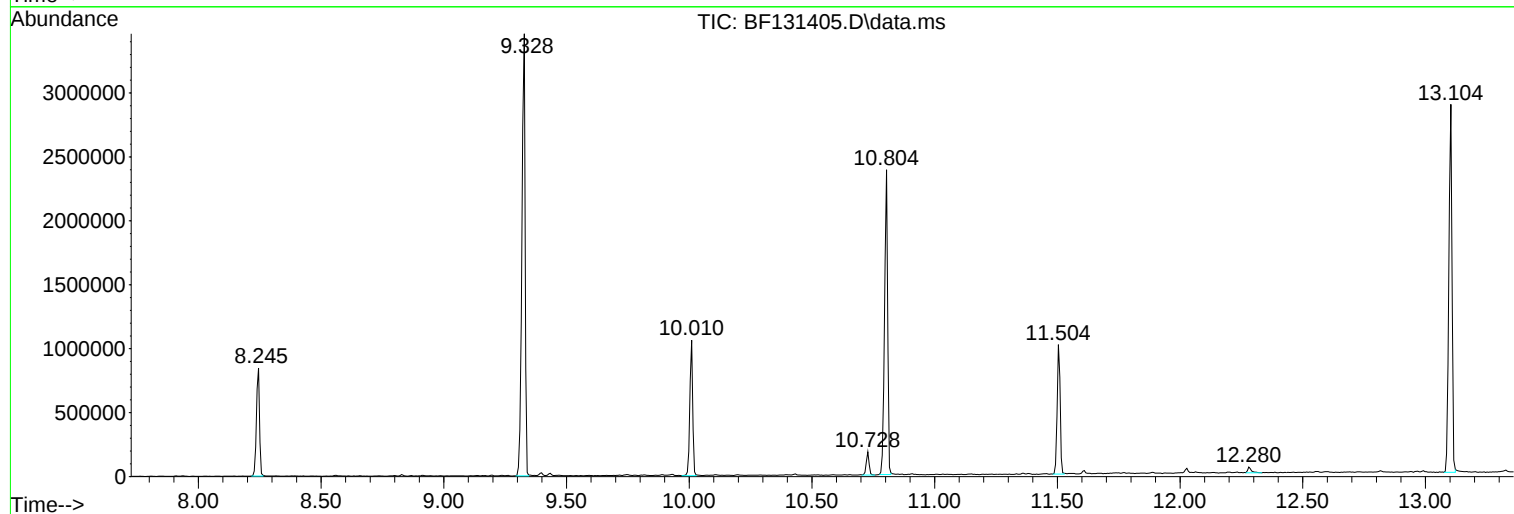
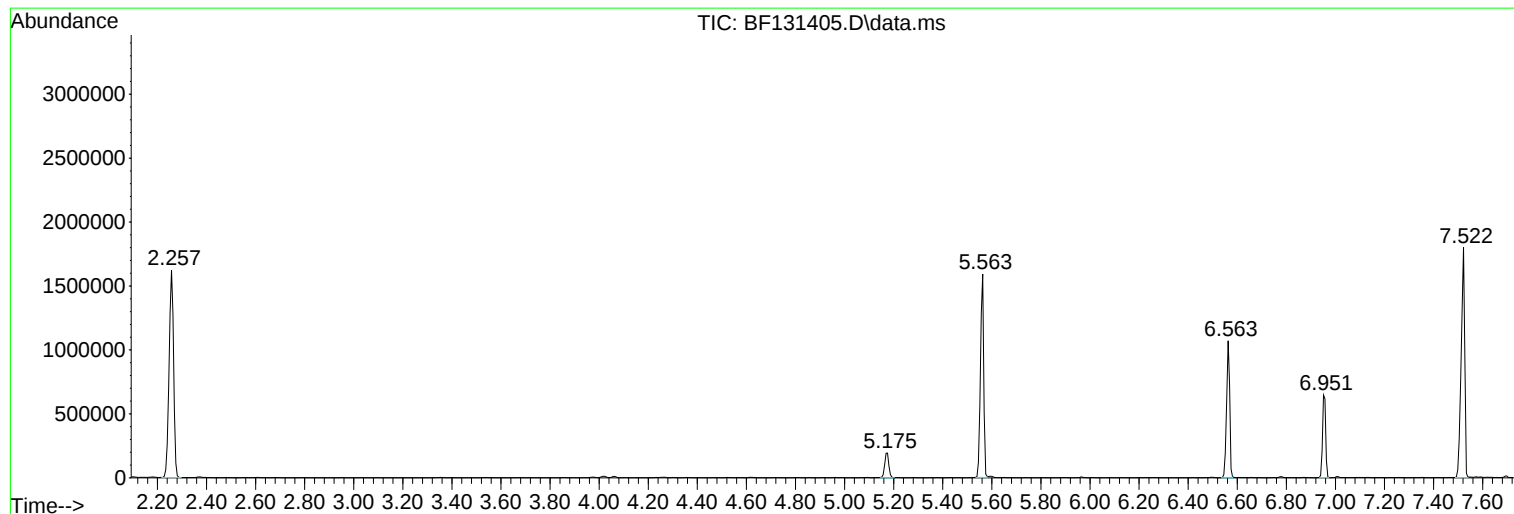
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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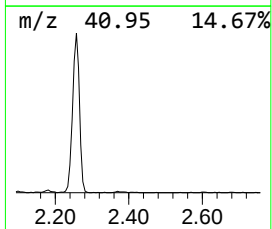
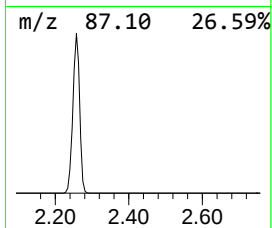
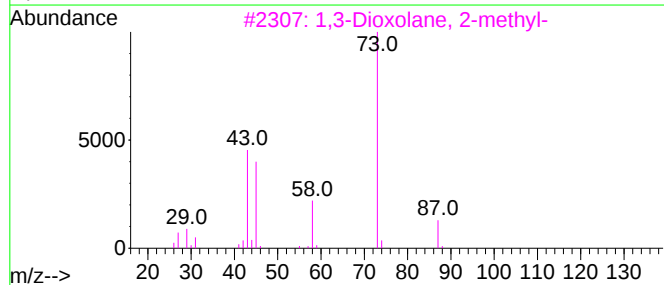
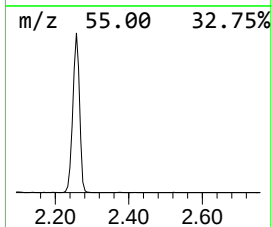
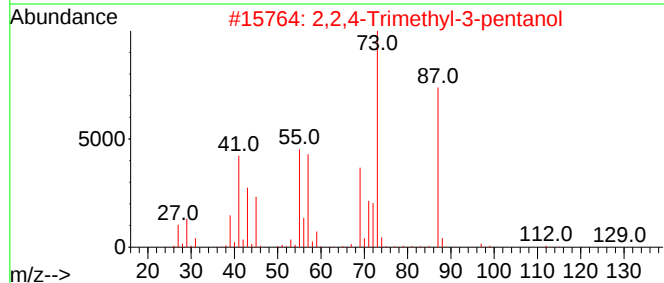
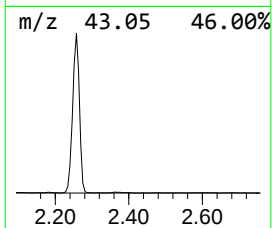
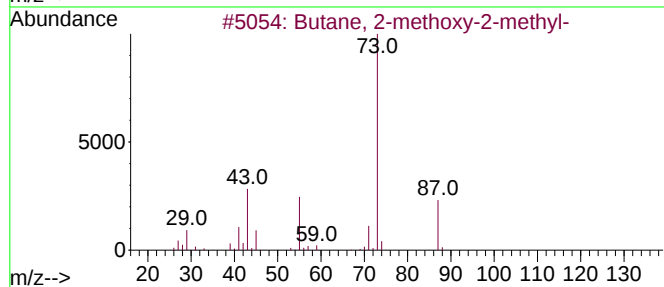
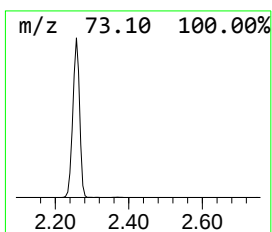
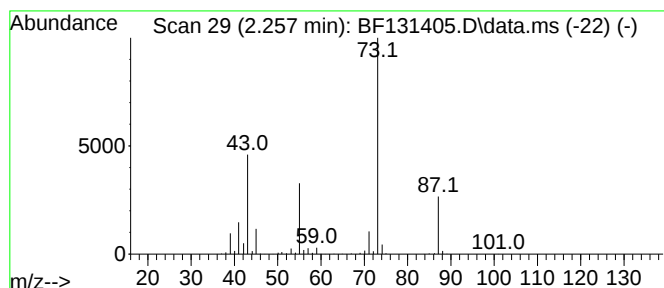
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.257	72.13 ng	2067880	1,4-Dichlorobenzene-d4	6.957

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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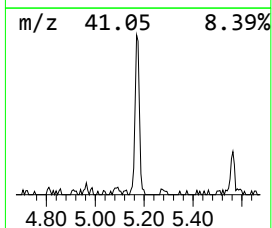
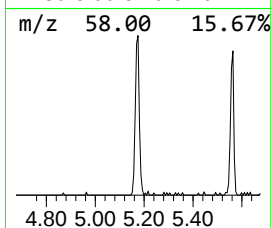
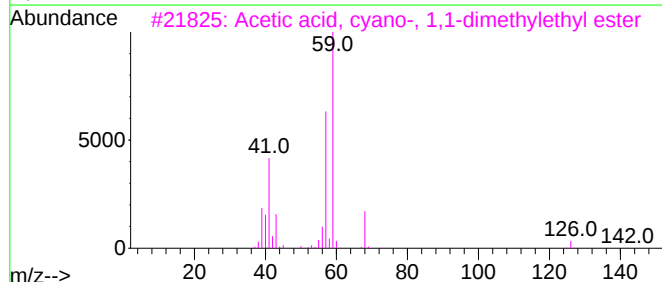
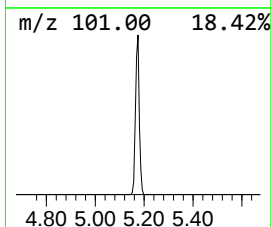
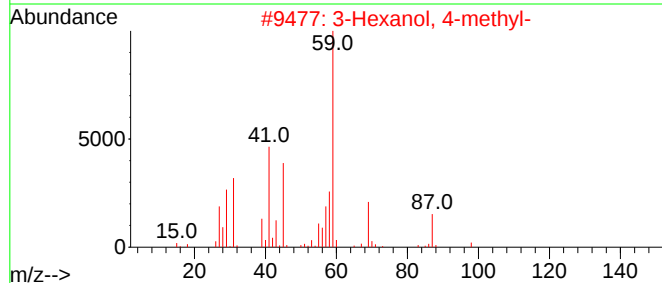
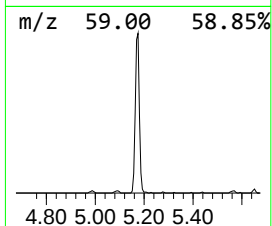
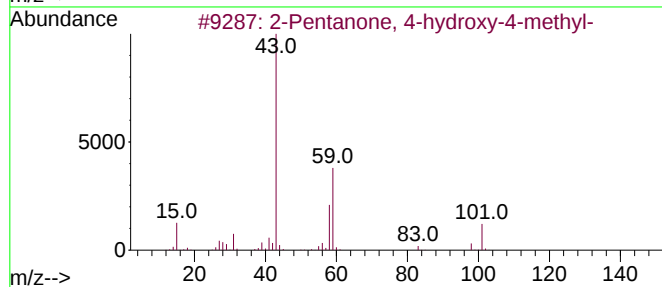
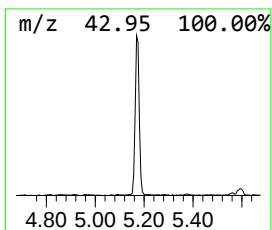
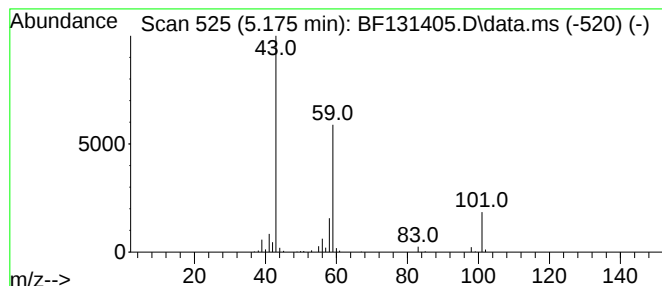
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	7.77 ng	222675	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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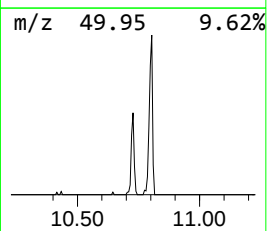
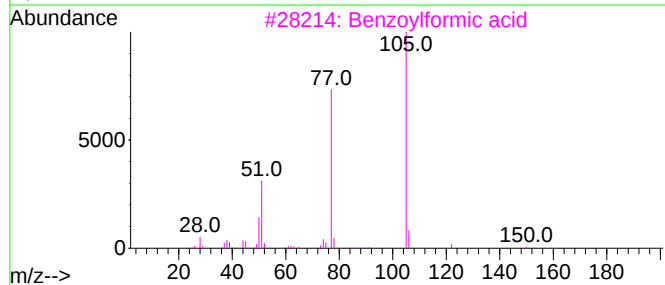
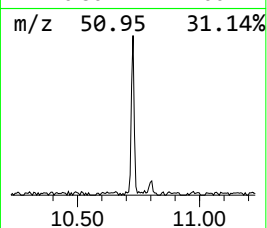
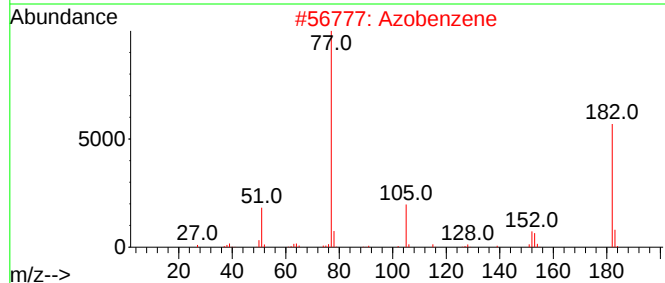
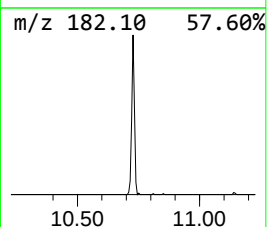
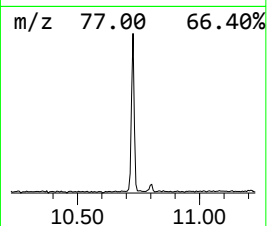
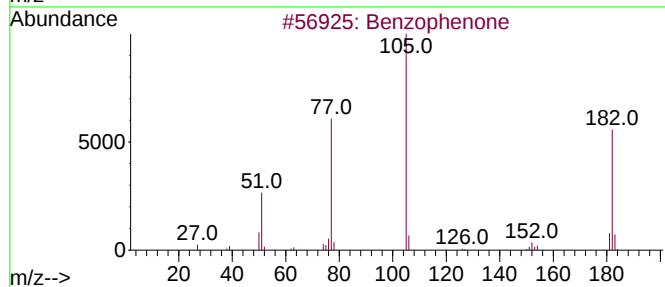
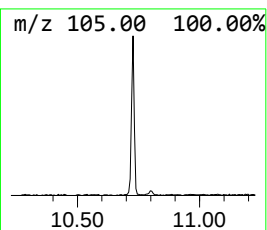
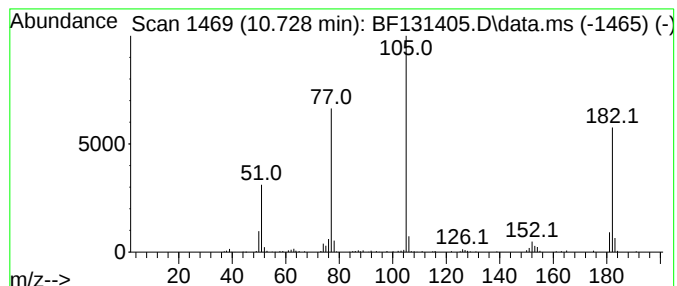
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.727	3.32 ng	142303	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	52
3			Benzoylformic acid	150	C8H6O3	000611-73-4	49
4			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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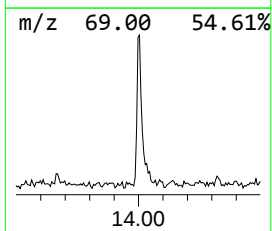
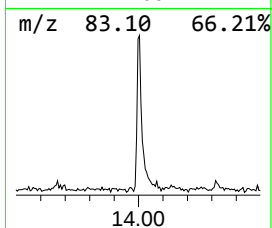
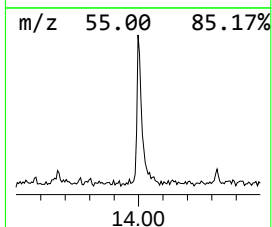
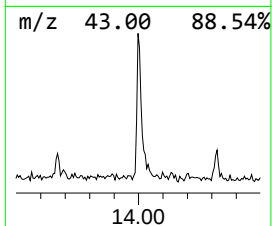
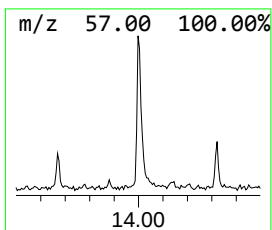
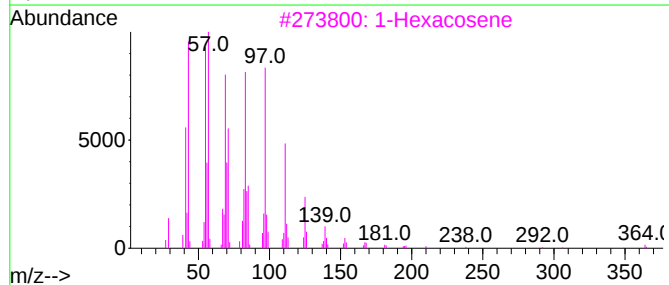
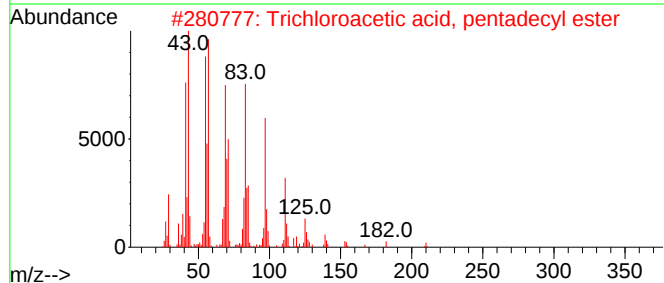
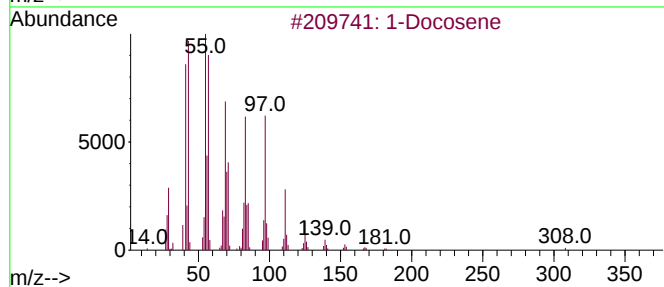
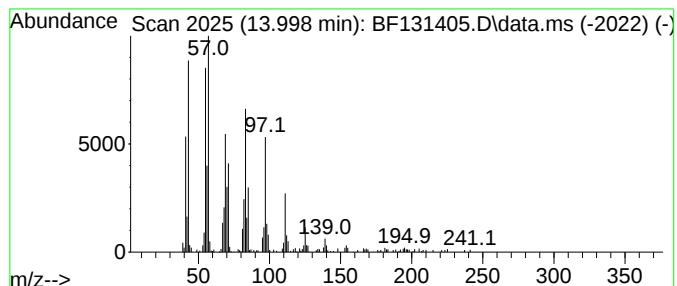
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	7.98 ng	227183	Chrysene-d12	14.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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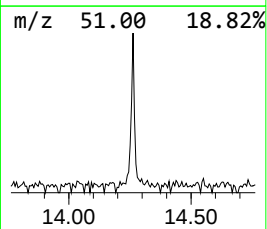
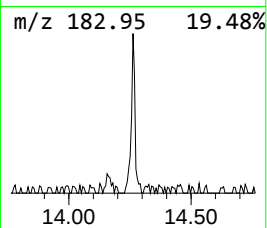
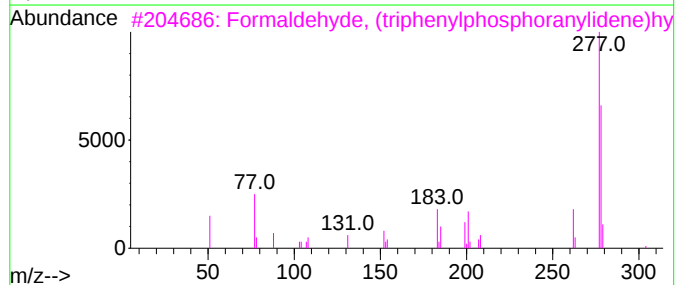
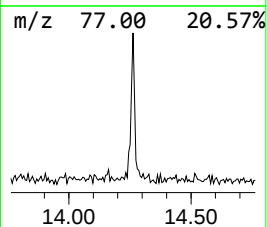
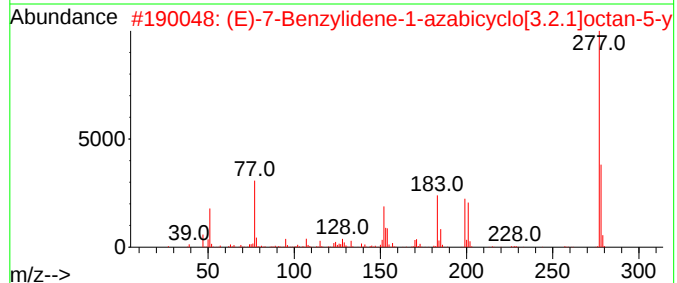
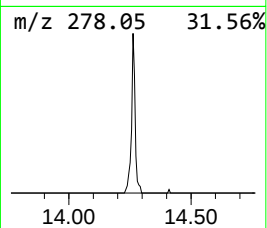
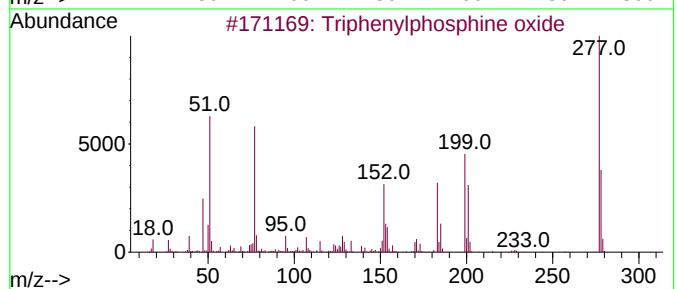
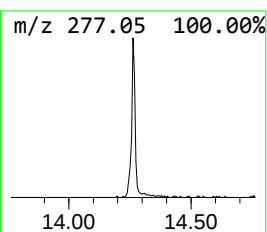
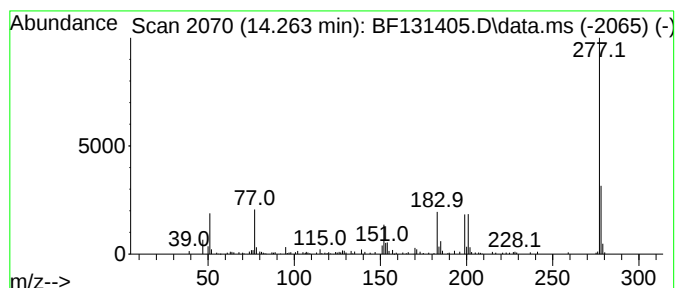
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	3.22 ng	91717	Chrysene-d12	14.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	83
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	59
4			Fenitrothion	277	C9H12N05PS	000122-14-5	32
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	28



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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...	2.257	72.1	ng	2067880	1	6.957	573376	20.0
2-Pentanone, 4-...	5.175	7.8	ng	222675	1	6.957	573376	20.0
Benzophenone	10.727	3.3	ng	142303	3	10.010	856795	20.0
1-Docosene	13.998	8.0	ng	227183	5	14.163	569442	20.0
Triphenylphosph...	14.263	3.2	ng	91717	5	14.163	569442	20.0