

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
 Data File : BF127716.D
 Acq On : 08 Apr 2022 16:27
 Operator : CG\JU
 Sample : N2317-13
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NORTH-5

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.352	3	11	17	rVB	329114	435199	10.99%	1.545%
2	2.463	23	30	36	rBV	53970	68020	1.72%	0.242%
3	5.210	488	497	507	rBV	165977	212200	5.36%	0.753%
4	5.587	555	561	564	rBV	3196998	3161329	79.82%	11.225%
5	6.581	723	730	733	rBV	2871636	3317301	83.76%	11.779%
6	6.963	791	795	798	rBV	1089615	868472	21.93%	3.084%
7	7.528	885	891	894	rBV	2117265	2194024	55.40%	7.790%
8	8.245	1008	1013	1017	rBV	1291324	1132431	28.59%	4.021%
9	9.328	1190	1197	1200	rBV	3765758	3880112	97.97%	13.777%
10	9.981	1303	1308	1309	rBV	195046	182104	4.60%	0.647%
11	10.010	1309	1313	1316	rVB	1490447	1322273	33.39%	4.695%
12	10.798	1438	1447	1450	rBV	2991880	2835603	71.60%	10.069%
13	11.498	1562	1566	1570	rBV	1572662	1450706	36.63%	5.151%
14	12.016	1650	1654	1659	rBV	114489	117699	2.97%	0.418%
15	13.092	1832	1837	1840	rBV	4241906	3960342	100.00%	14.062%
16	13.851	1963	1966	1970	rBV	158819	129309	3.27%	0.459%
17	13.986	1985	1989	2009	rBV	308676	571859	14.44%	2.031%
18	14.151	2013	2017	2020	rVV	1161126	1070437	27.03%	3.801%
19	14.245	2023	2033	2046	rBV3	157704	389391	9.83%	1.383%
20	14.633	2096	2099	2108	rVB6	28217	50903	1.29%	0.181%
21	15.674	2270	2276	2290	rVB	635160	813378	20.54%	2.888%

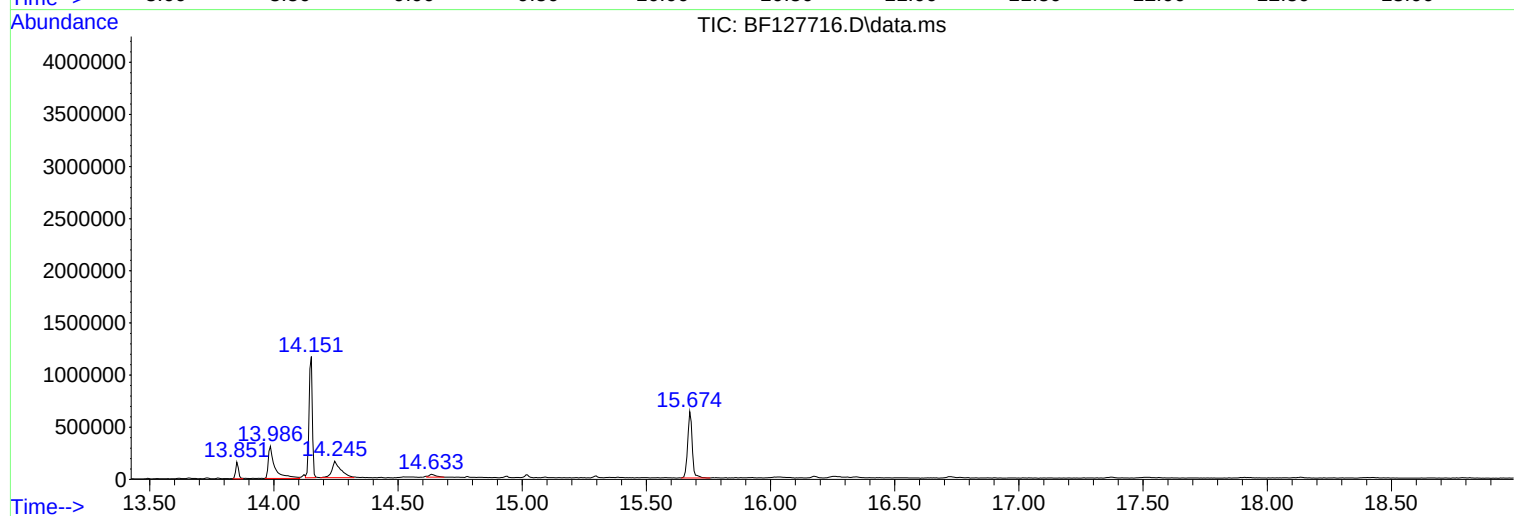
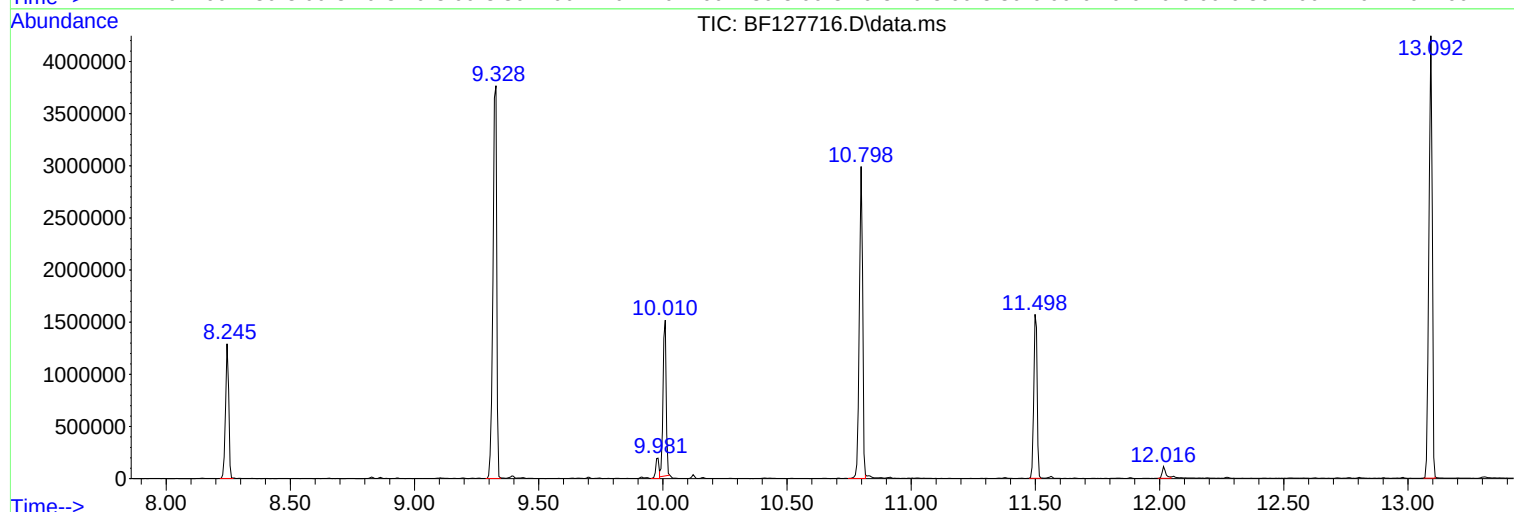
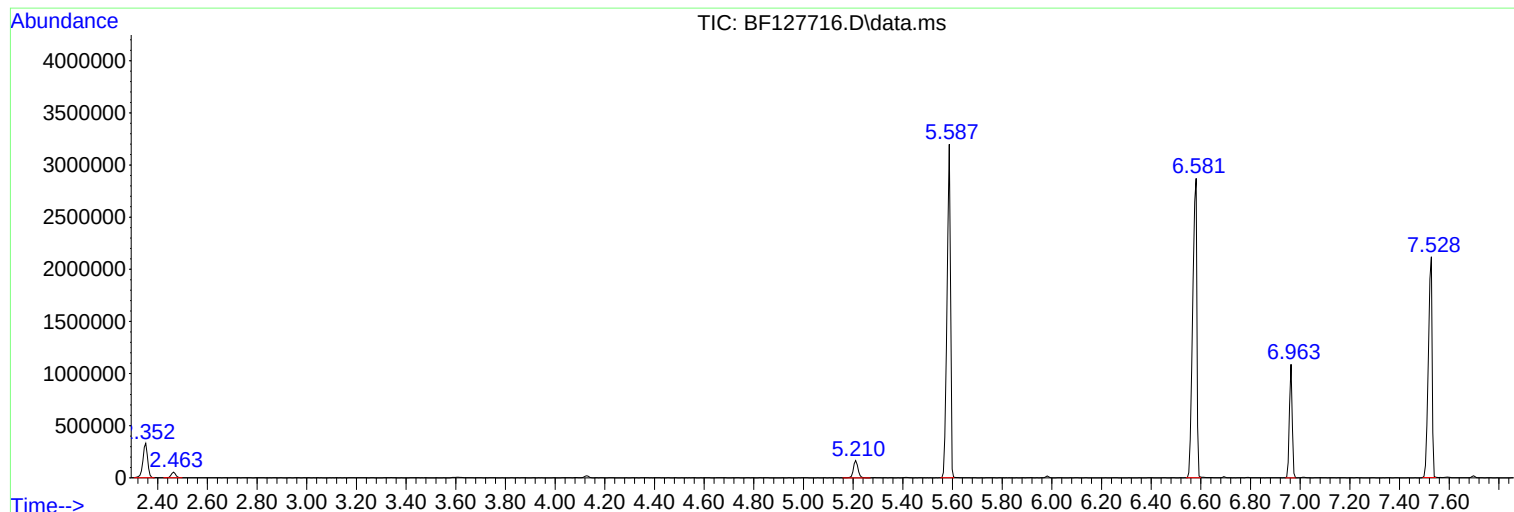
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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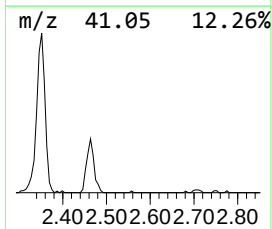
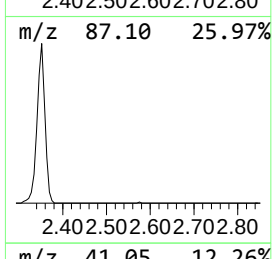
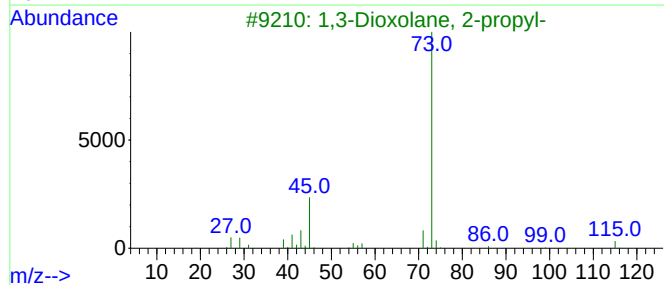
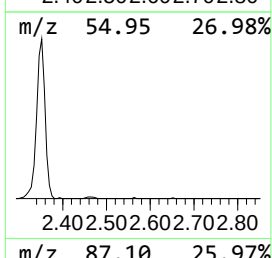
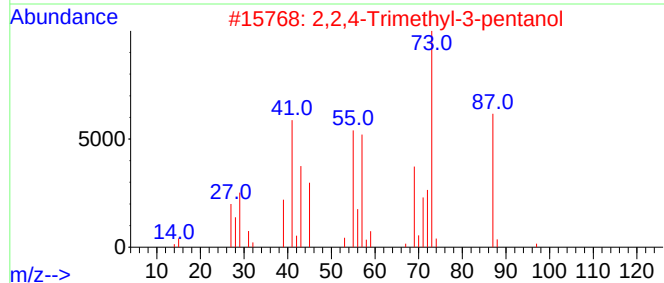
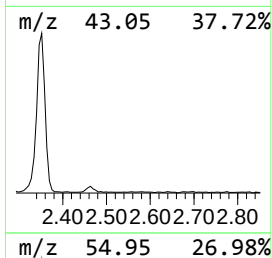
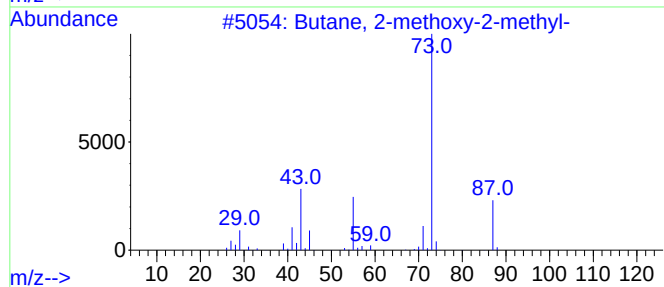
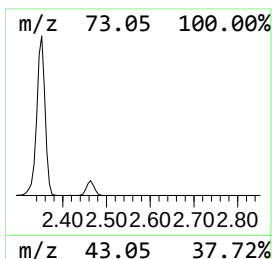
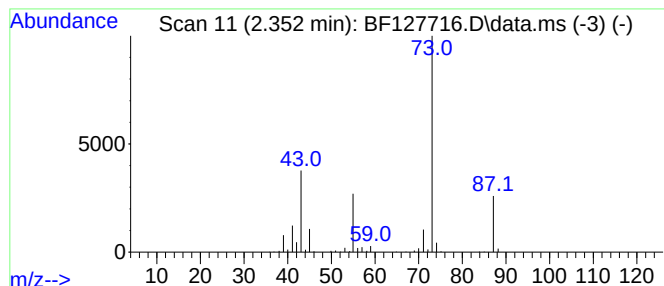
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.352	10.02 ng	435199	1,4-Dichlorobenzene-d4	6.963

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-propyl-	116	C6H12O2	003390-13-4	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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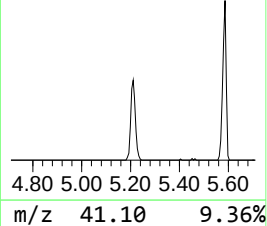
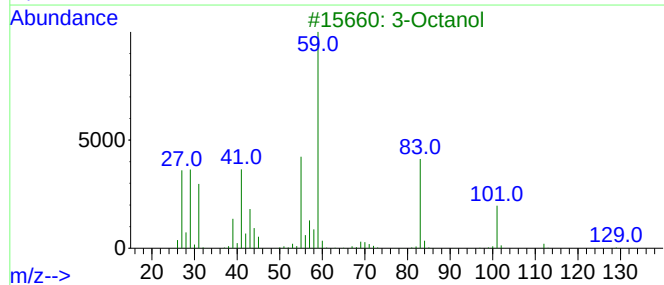
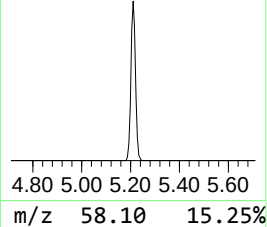
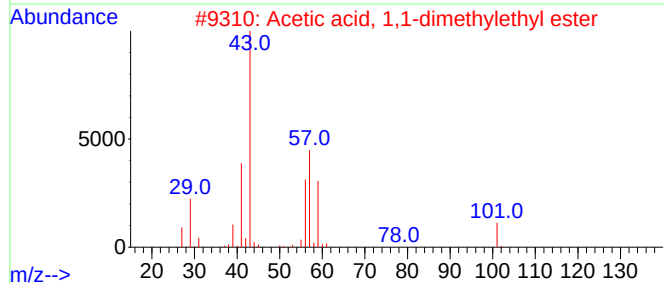
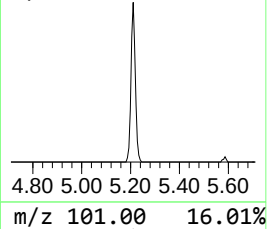
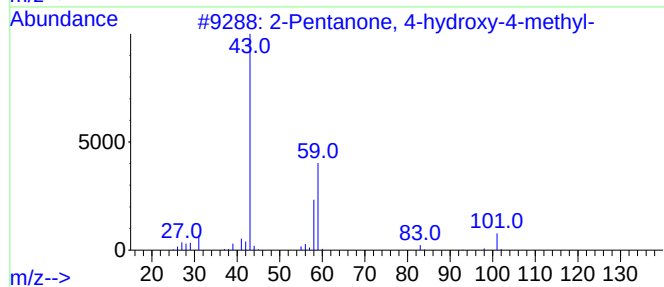
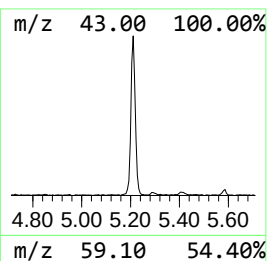
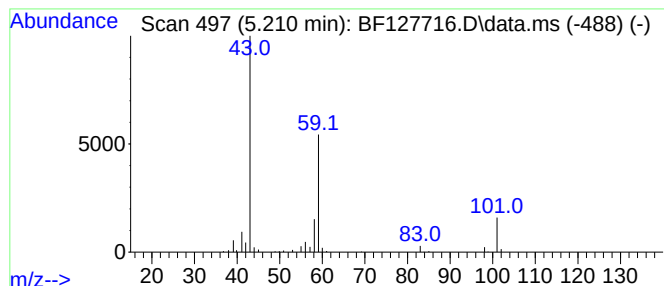
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.210	4.89 ng	212200	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Octanol	130	C8H18O	000589-98-0	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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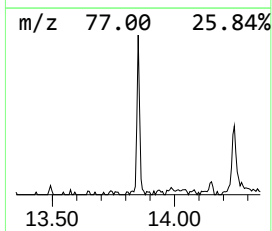
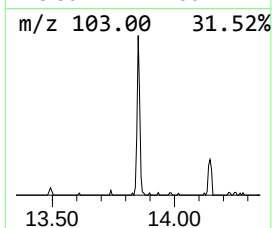
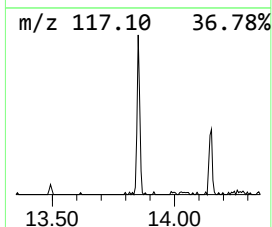
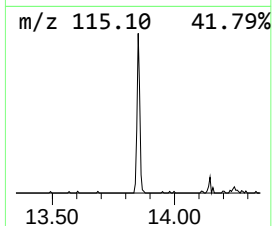
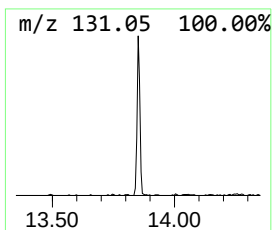
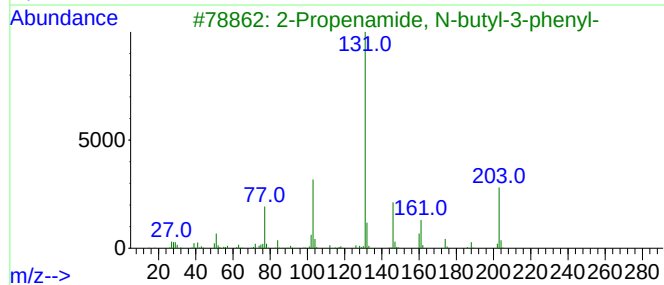
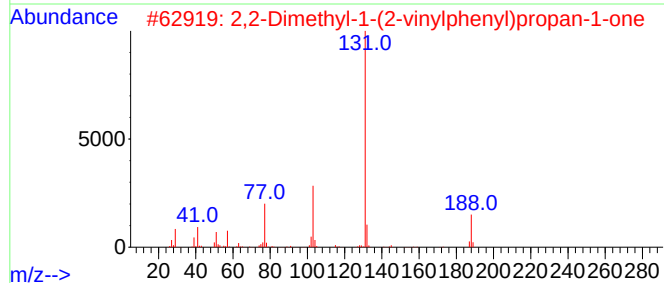
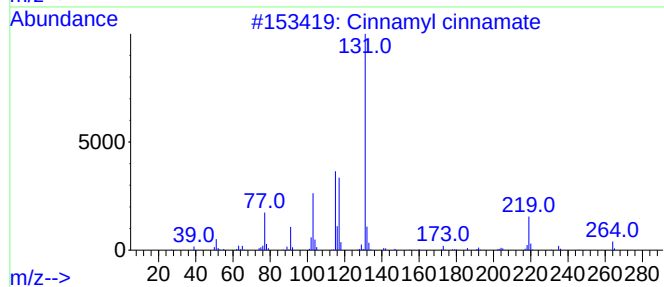
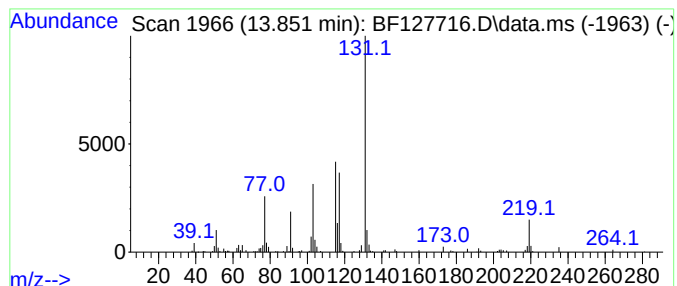
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	2.42 ng	129309	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49
3			2-Propenamide, N-butyl-3-phenyl-	203	C13H17NO	006299-56-5	47
4			2-Propenamide, N,N-diethyl-3-phe...	203	C13H17NO	003680-04-4	47
5			2,4,5-Trichlorophenyl cinnamate	326	C15H9Cl3O2	1010242-39-6	47



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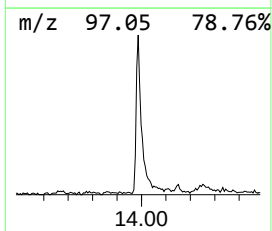
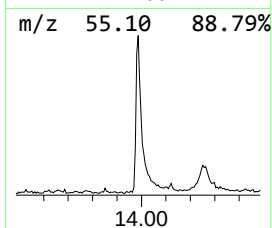
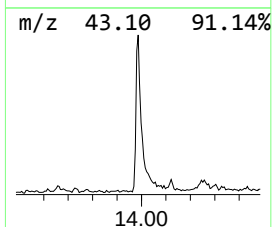
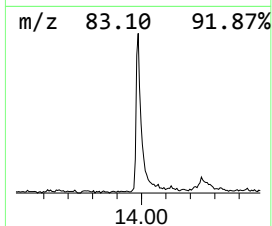
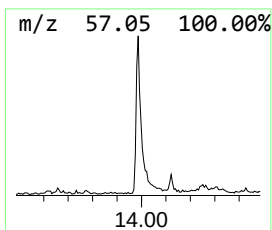
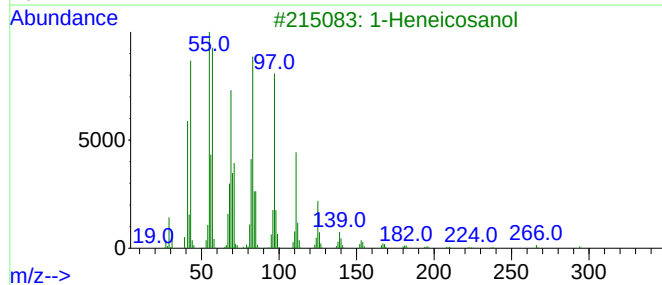
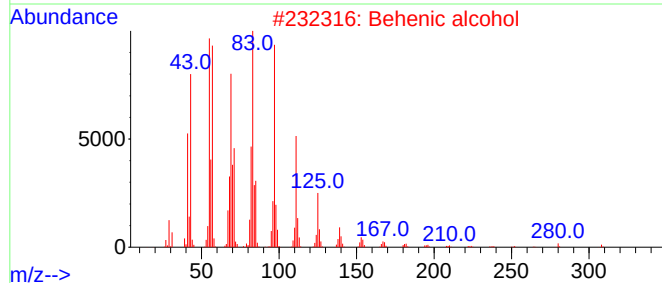
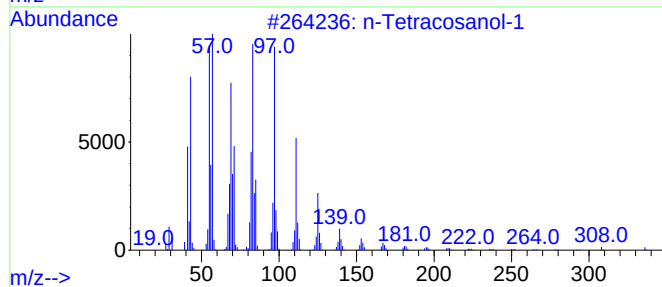
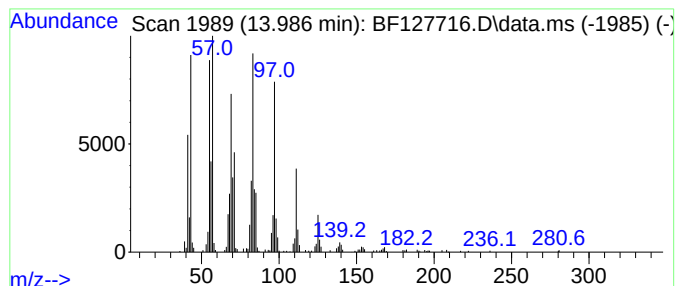
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.986	10.68 ng	571859	Chrysene-d12	14.151	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	1-Tricosene	322	C23H46	018835-32-0	91



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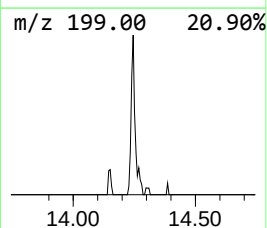
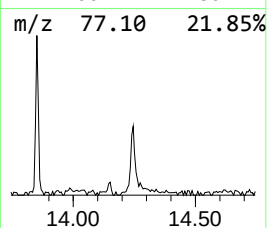
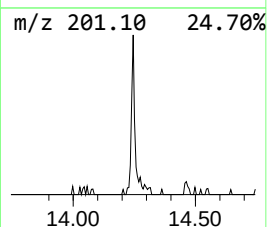
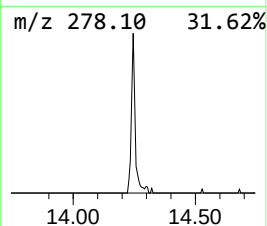
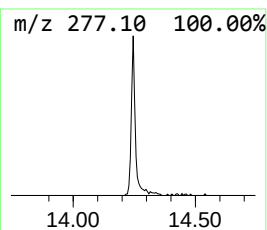
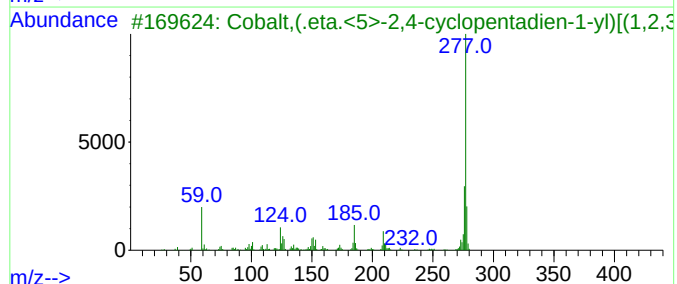
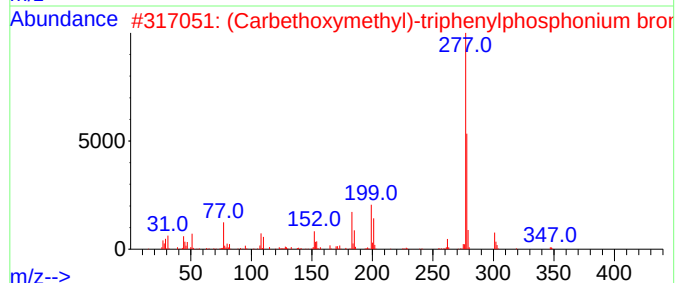
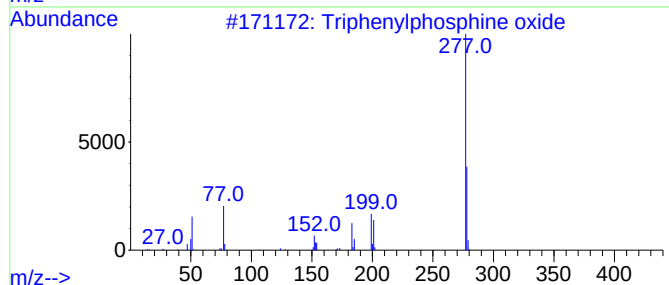
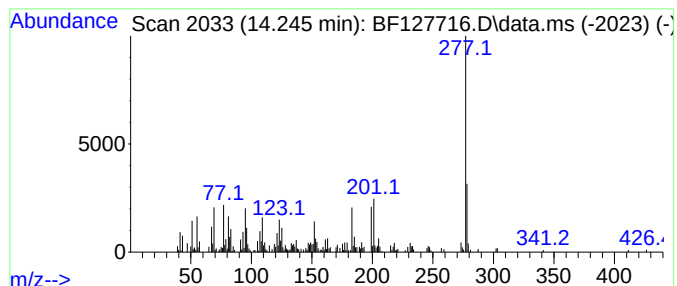
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	7.28 ng	389391	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	70
2			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	53
3			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
4			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	38
5			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.352	10.0	ng	435199	1	6.963	868472	20.0
2-Pentanone, 4-...	5.210	4.9	ng	212200	1	6.963	868472	20.0
Cinnamyl cinnamate	13.851	2.4	ng	129309	5	14.151	1070440	20.0
n-Tetracosanol-1	13.986	10.7	ng	571859	5	14.151	1070440	20.0
Triphenylphosph...	14.245	7.3	ng	389391	5	14.151	1070440	20.0