

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
 Data File : BM047299.D
 Acq On : 21 Aug 2024 15:46
 Operator : RC/JU
 Sample : P3580-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 926-K1-SD-0.5-1-081224

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_M\Methods\8270-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047299.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	60	63	77	rBV	67176	120608	2.16%	0.348%
2	4.563	280	285	294	rBV	99875	142008	2.55%	0.409%
3	5.010	355	361	372	rBV	1707213	2530504	45.42%	7.296%
4	6.569	618	626	642	rBV	1601764	2592194	46.53%	7.474%
5	7.351	752	759	769	rBV	723486	1133249	20.34%	3.268%
6	8.498	947	954	969	rBV	1000383	1686447	30.27%	4.863%
7	10.110	1219	1228	1242	rBV	897958	1495891	26.85%	4.313%
8	10.875	1352	1358	1368	rBV	76444	164956	2.96%	0.476%
9	12.622	1648	1655	1672	rBV	2342808	3643231	65.40%	10.505%
10	14.016	1885	1892	1910	rBV	1369461	2079681	37.33%	5.996%
11	14.269	1926	1935	1941	rBV4	50660	116974	2.10%	0.337%
12	15.521	2142	2148	2175	rBV	2032753	3360512	60.32%	9.690%
13	16.780	2351	2362	2377	rBV	1804717	2700058	48.47%	7.785%
14	17.715	2516	2521	2529	rBV2	207440	330177	5.93%	0.952%
15	18.857	2711	2715	2720	rBV	87836	127781	2.29%	0.368%
16	19.015	2738	2742	2750	rBV2	82954	145769	2.62%	0.420%
17	19.227	2774	2778	2783	rVB	66388	93551	1.68%	0.270%
18	19.445	2810	2815	2830	rBV	4541987	5570880	100.00%	16.063%
19	20.756	3034	3038	3044	rBV2	240745	391320	7.02%	1.128%
20	21.021	3077	3083	3095	rBV	2263149	3274050	58.77%	9.440%
21	23.715	3534	3541	3556	rVB	1269501	2981792	53.52%	8.598%

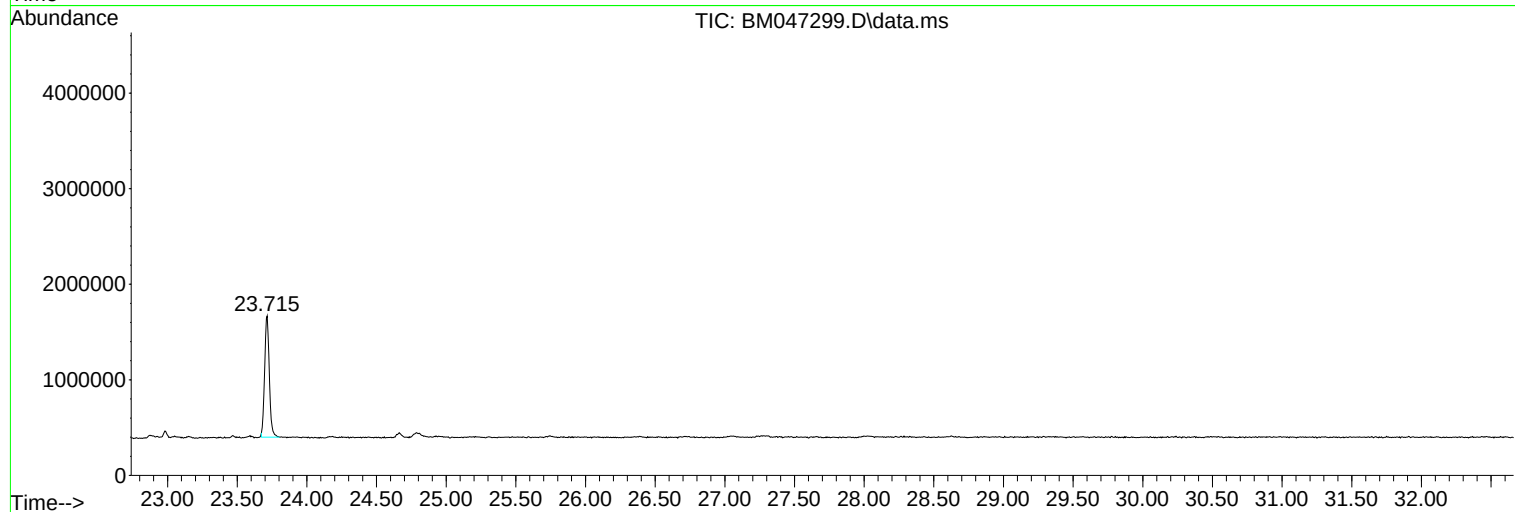
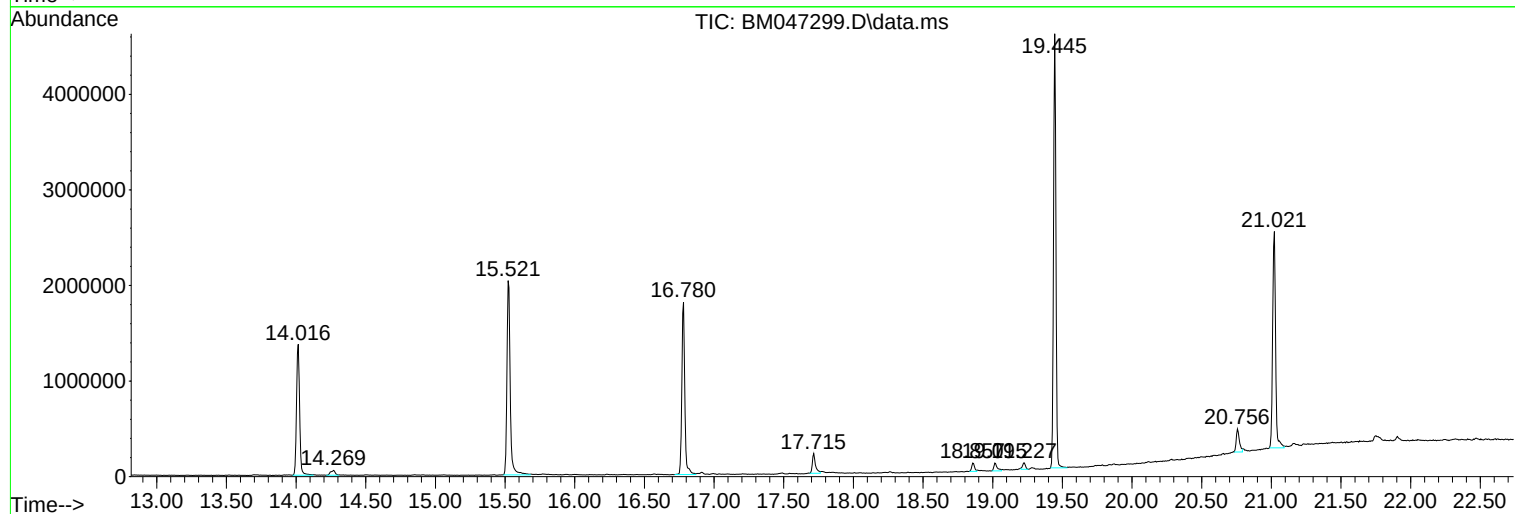
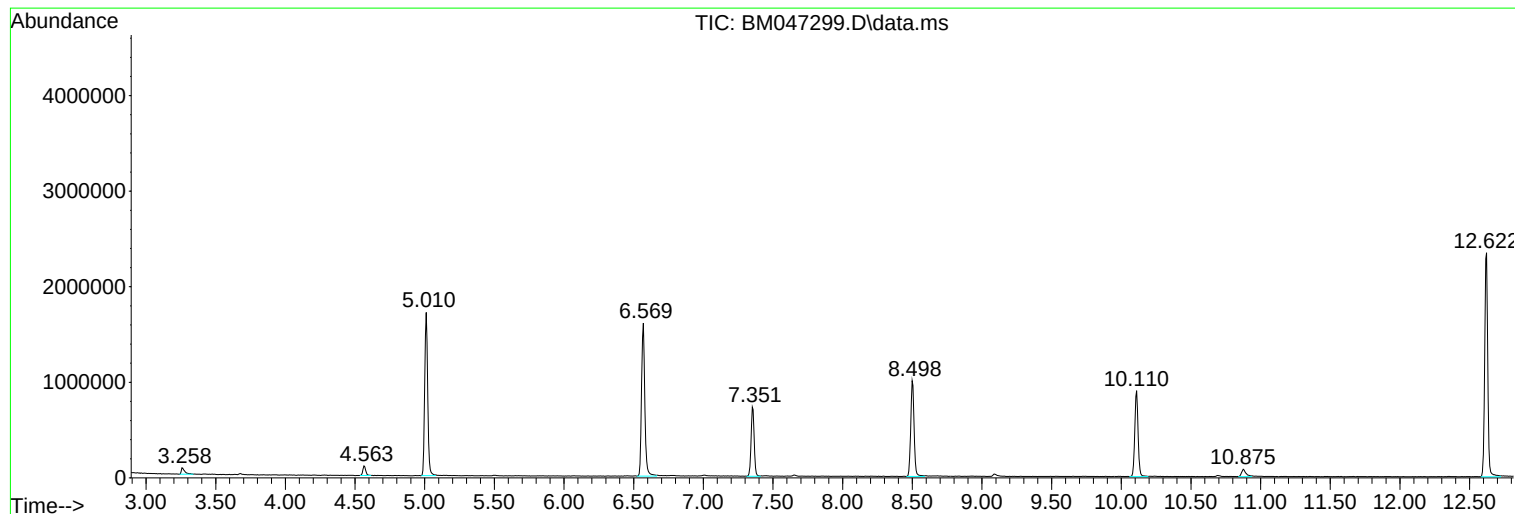
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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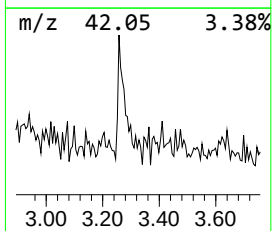
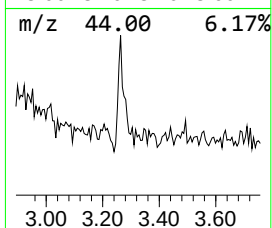
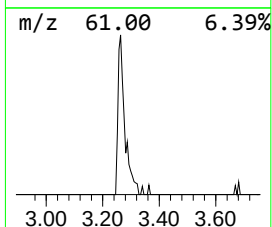
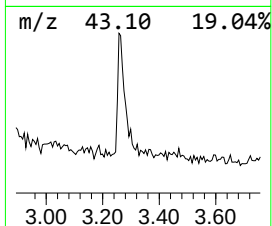
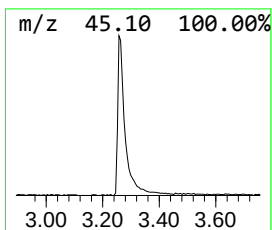
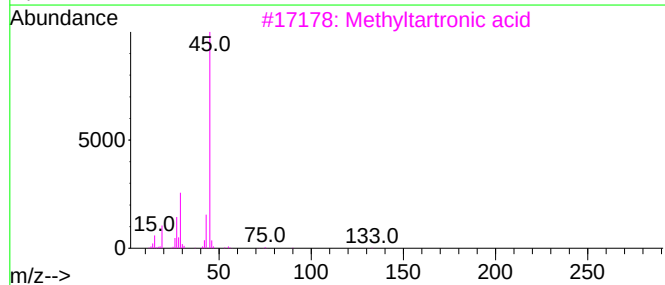
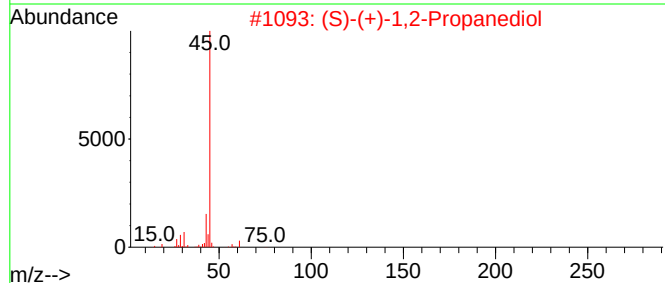
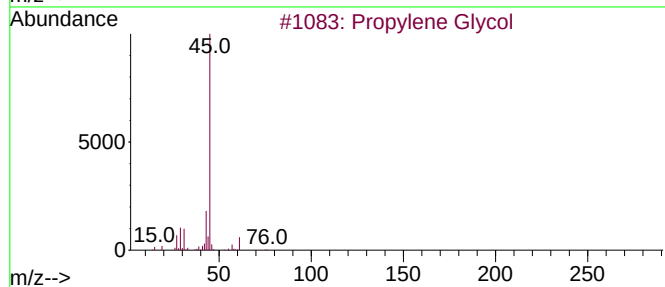
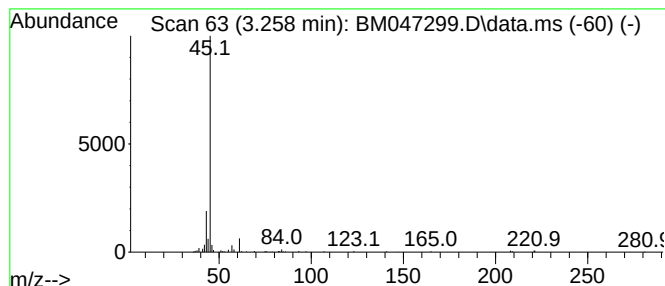
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	2.13 ng	120608	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	80
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3			Methyltartronic acid	134	C4H6O5	000595-98-2	9
4			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
5			L-Lactic acid	90	C3H6O3	000079-33-4	9



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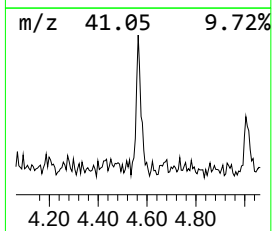
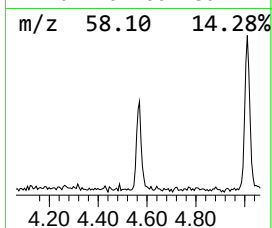
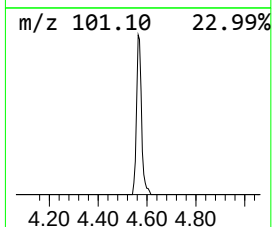
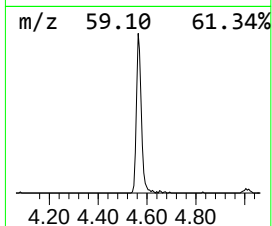
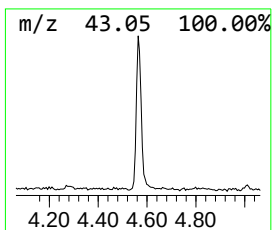
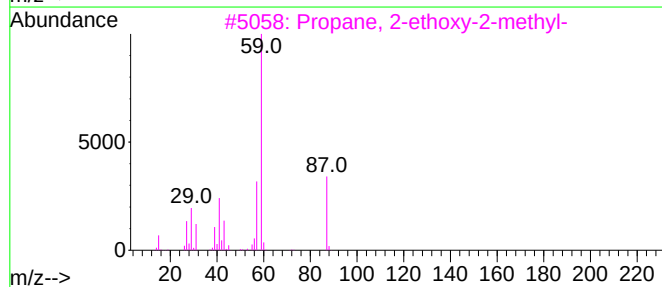
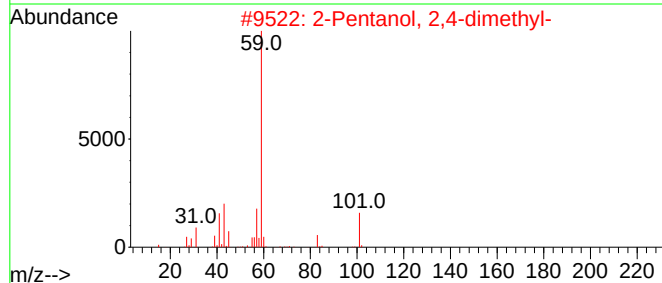
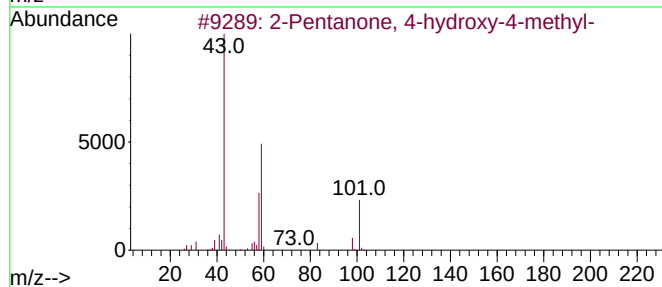
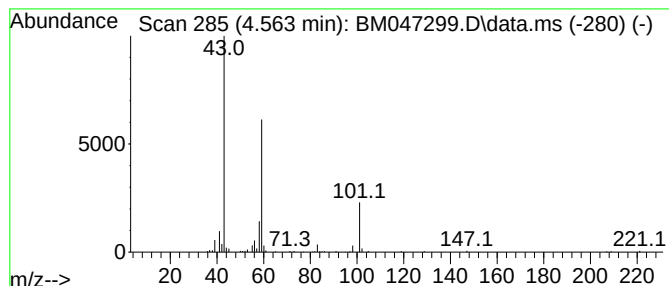
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	2.51 ng	142008	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	25
4			1,2-Butanediol	90	C4H10O2	000584-03-2	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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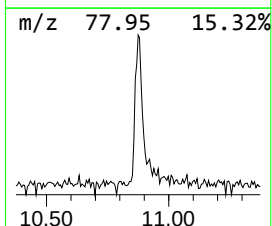
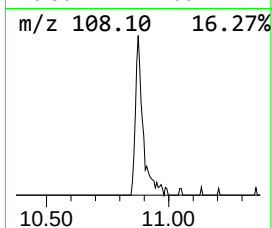
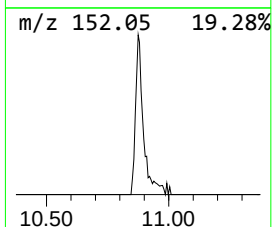
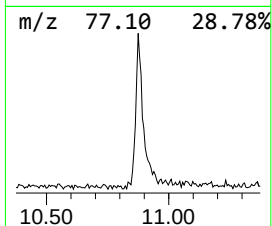
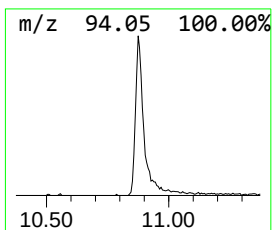
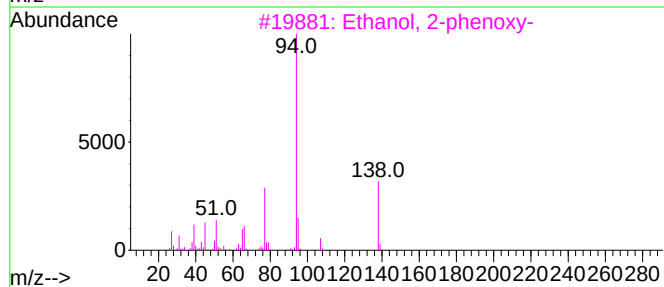
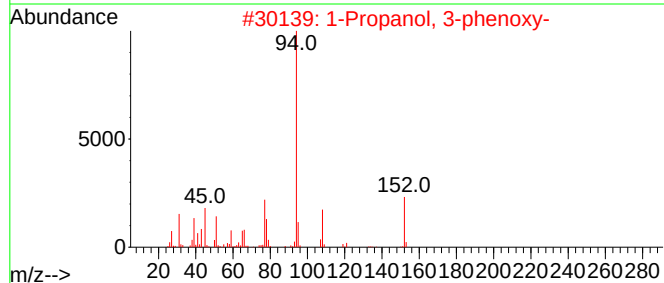
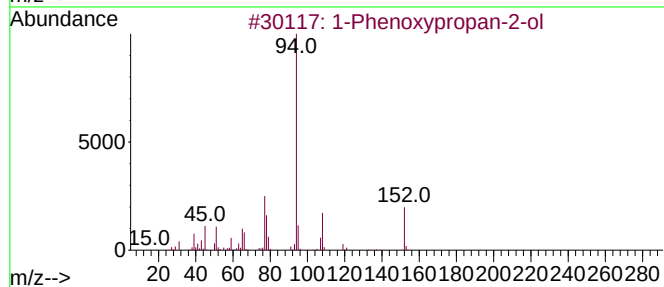
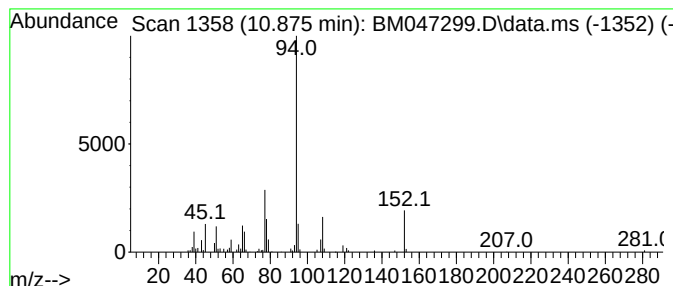
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.21 ng	164956	Naphthalene-d8	10.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4			1-Amino-3-phenoxypropan-2-ol	167	C9H13NO2	004287-19-8	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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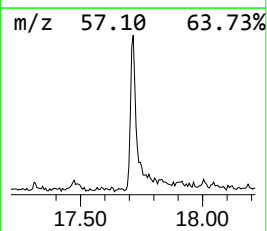
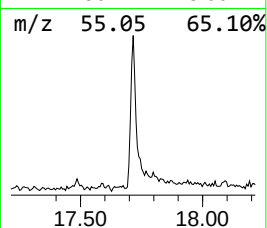
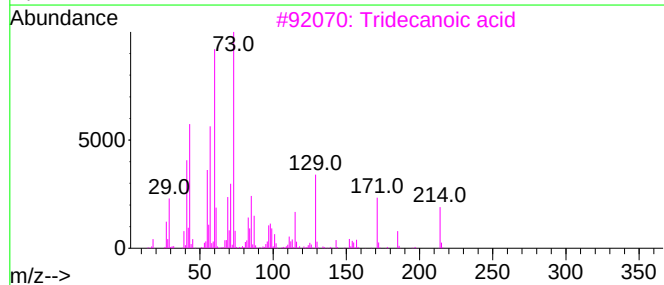
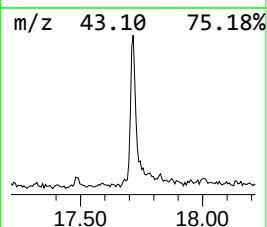
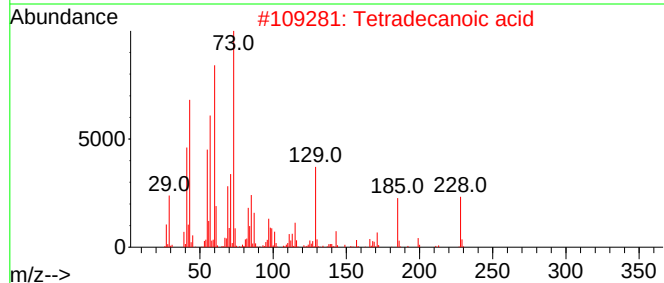
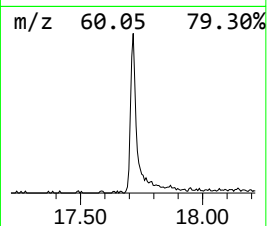
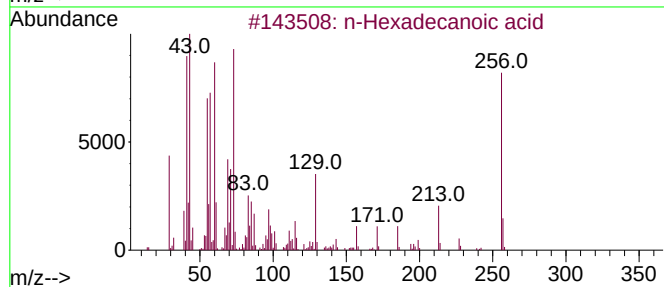
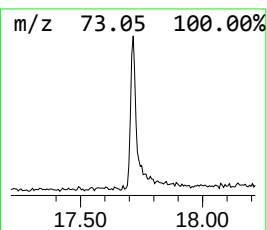
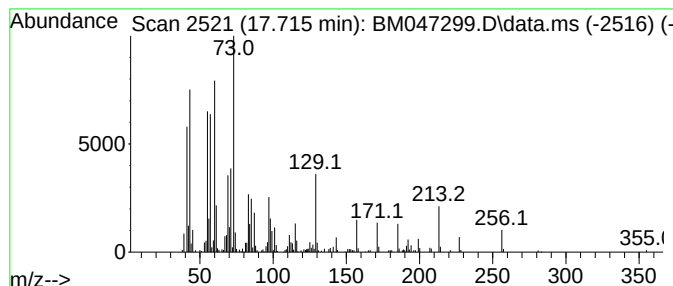
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	2.45 ng	330177	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	81



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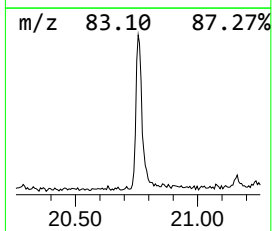
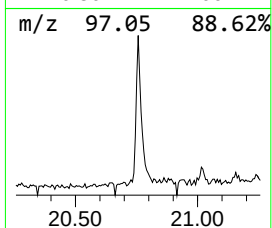
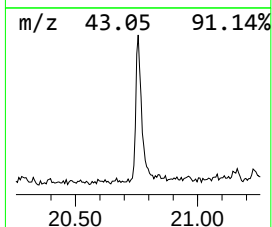
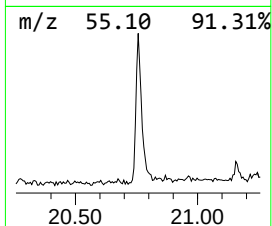
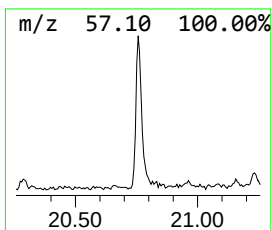
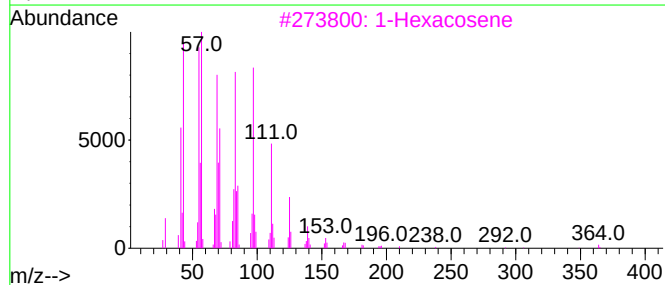
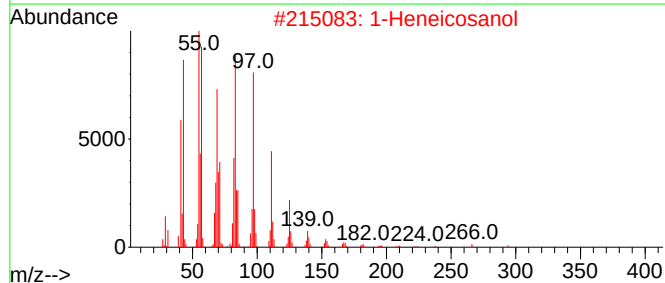
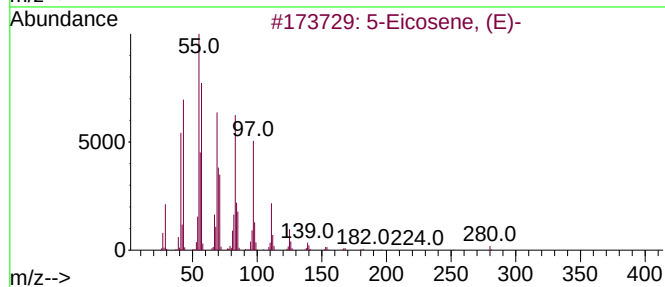
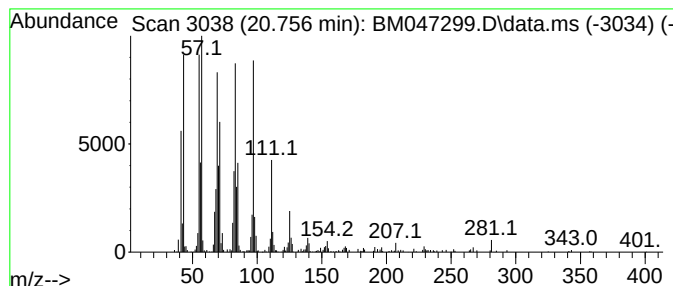
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	2.39 ng	391320	Chrysene-d12	21.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		1-Hexacosene	364	C26H52	018835-33-1	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	91
5		Pentacos-1-ene	350	C25H50	016980-85-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.258	2.1	ng	120608	1	7.351	1133250	20.0
2-Pentanone, 4-...	4.563	2.5	ng	142008	1	7.351	1133250	20.0
1-Phenoxypropan...	10.875	2.2	ng	164956	2	10.110	1495890	20.0
n-Hexadecanoic ...	17.715	2.5	ng	330177	4	16.780	2700060	20.0
5-Eicosene, (E)-	20.756	2.4	ng	391320	5	21.021	3274050	20.0