

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
 Data File : BM047270.D
 Acq On : 20 Aug 2024 14:06
 Operator : RC/JU
 Sample : P3643-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 918-J-SD-0.5-1-081524

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: BM047270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.569	279	286	293	rBV	152436	216257	2.11%	0.419%
2	5.016	355	362	375	rBV	2654444	3902331	38.02%	7.570%
3	6.575	617	627	641	rBV	2679431	4206614	40.99%	8.160%
4	7.357	753	760	770	rVB	803742	1224463	11.93%	2.375%
5	8.504	948	955	969	rBV	1633459	2661313	25.93%	5.162%
6	10.116	1221	1229	1241	rBV	975407	1662495	16.20%	3.225%
7	10.880	1351	1359	1369	rBV	78782	176122	1.72%	0.342%
8	12.627	1649	1656	1676	rBV	3989584	6157604	59.99%	11.944%
9	14.015	1886	1892	1902	rBV	1520640	2335647	22.76%	4.531%
10	14.274	1927	1936	1949	rBV	932167	2011586	19.60%	3.902%
11	15.527	2142	2149	2162	rBV	3941145	5804179	56.55%	11.259%
12	16.786	2357	2363	2377	rBV	2009173	2962138	28.86%	5.746%
13	17.721	2517	2522	2527	rBV	358688	562909	5.48%	1.092%
14	19.021	2739	2743	2755	rBV	210371	367675	3.58%	0.713%
15	19.450	2810	2816	2825	rBV	8400811	10263576	100.00%	19.909%
16	20.762	3034	3039	3050	rBV2	401730	731056	7.12%	1.418%
17	21.021	3078	3083	3092	rBV2	2397109	3353781	32.68%	6.506%
18	23.721	3535	3542	3556	rVB	1265401	2953157	28.77%	5.728%

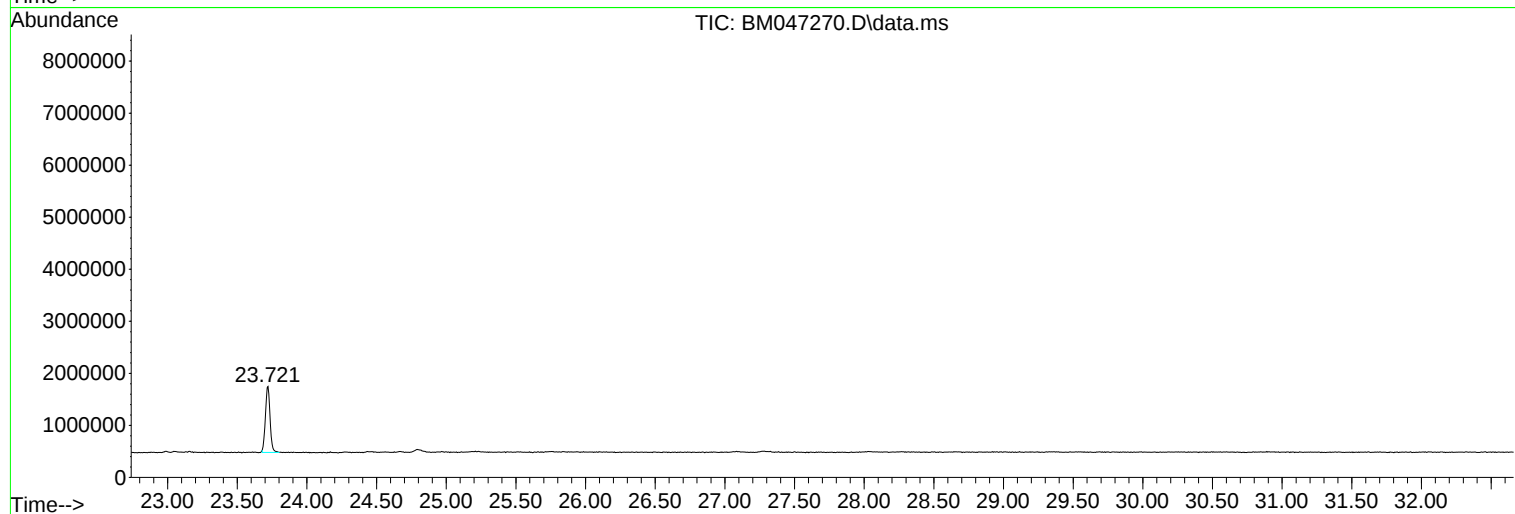
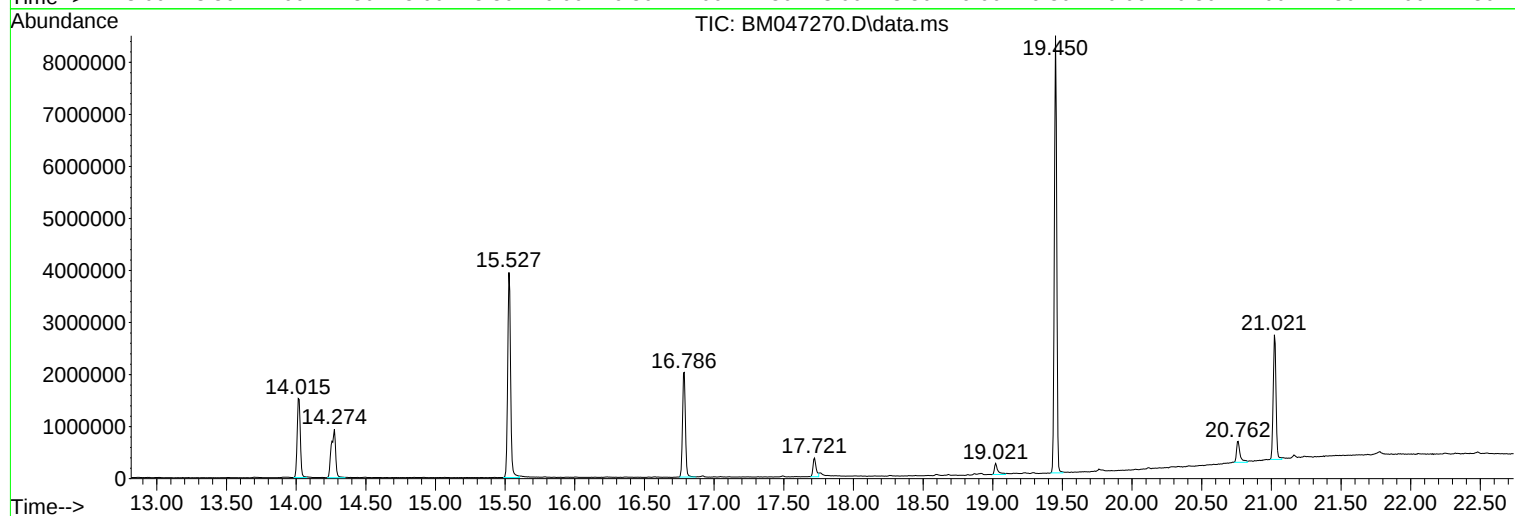
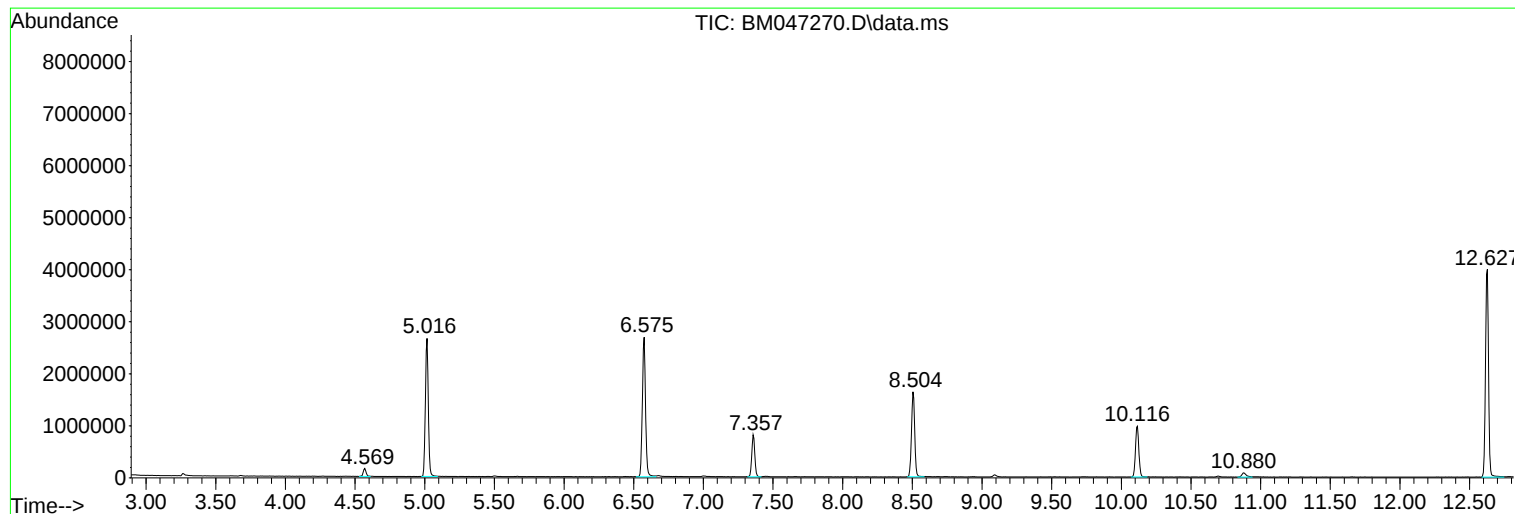
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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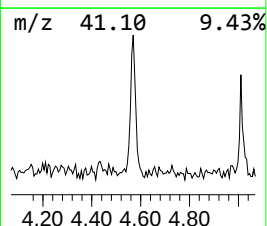
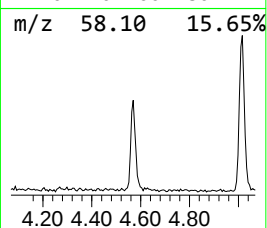
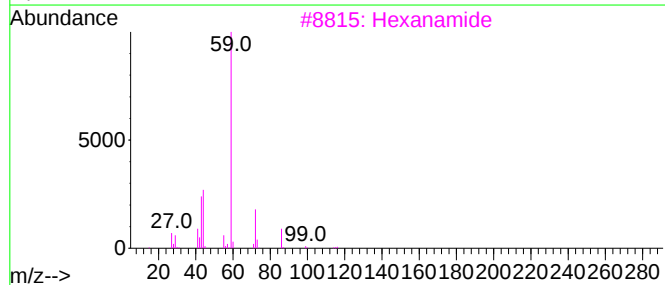
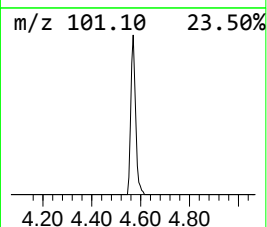
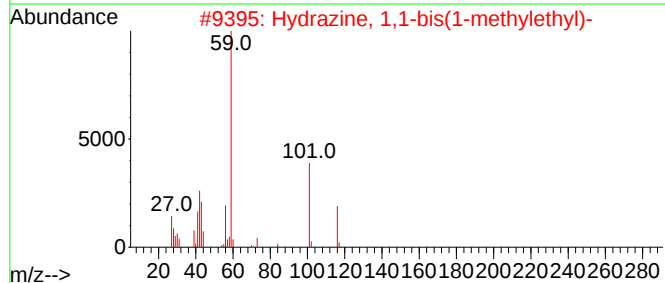
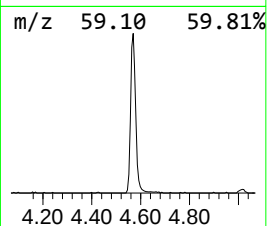
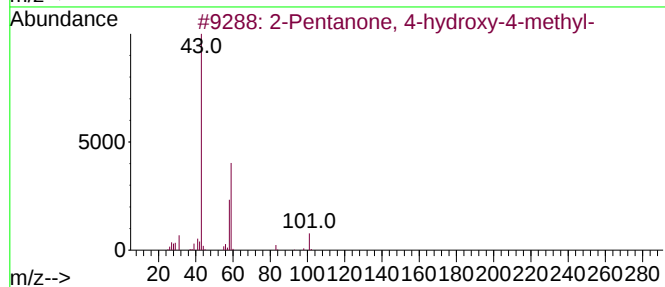
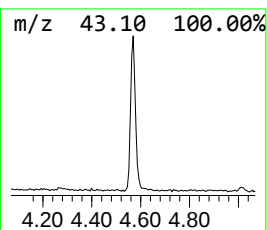
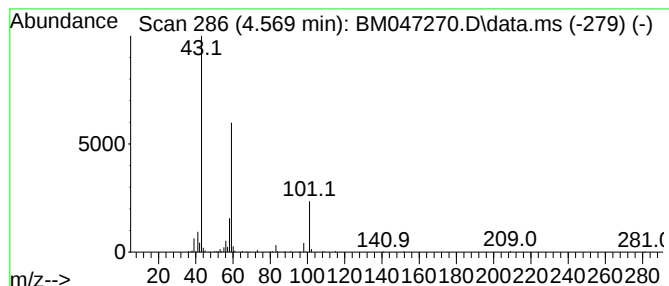
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.53 ng	216257	1,4-Dichlorobenzene-d4	7.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28	
3	Hexanamide	115	C6H13NO	000628-02-4	25	
4	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17	
5	1,2-Butanediol	90	C4H10O2	000584-03-2	17	



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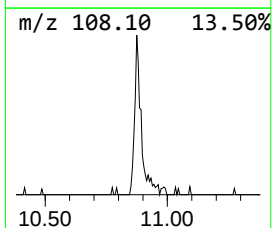
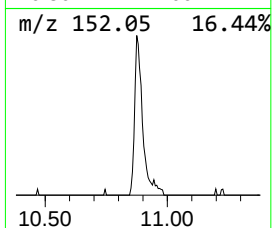
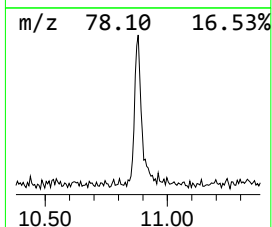
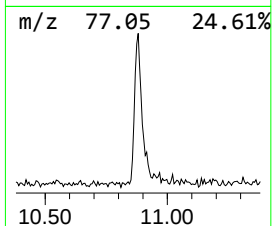
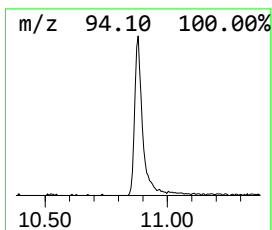
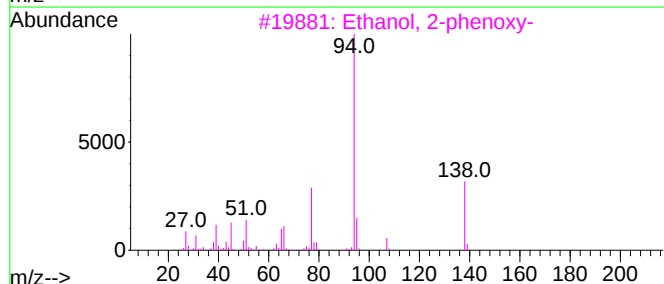
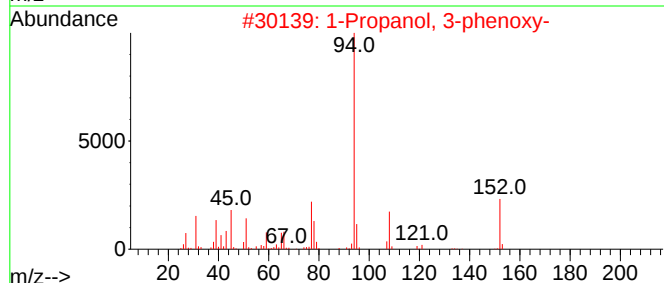
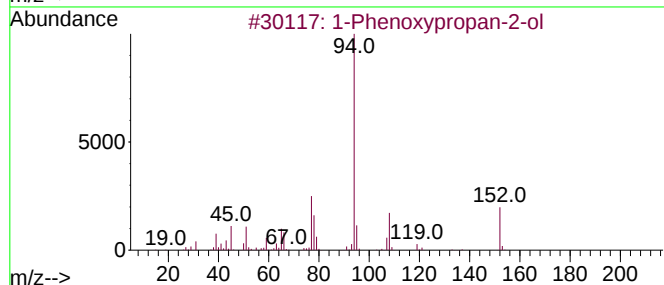
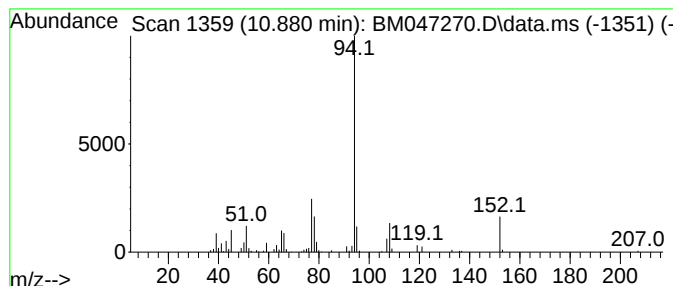
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.880	2.12 ng	176122	Naphthalene-d8	10.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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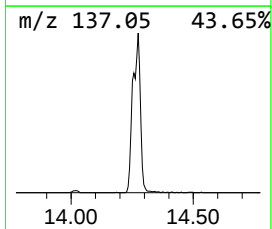
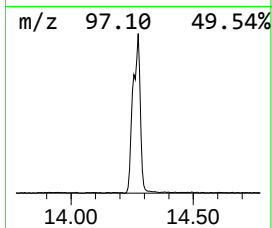
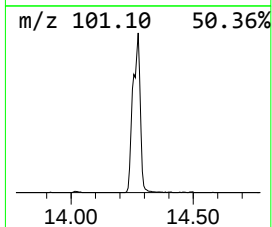
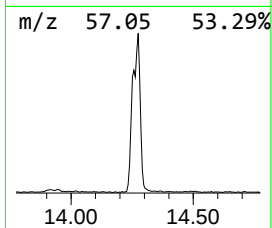
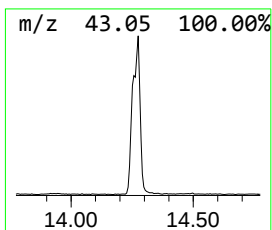
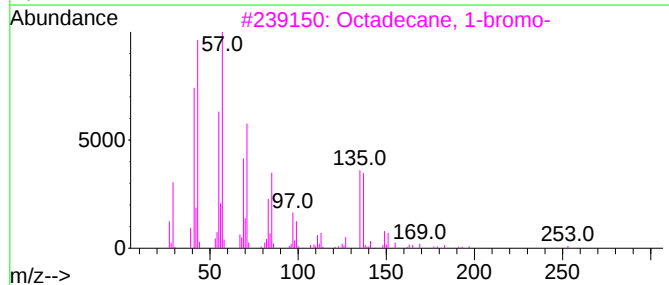
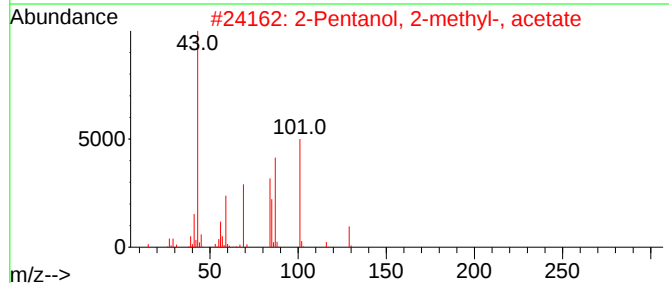
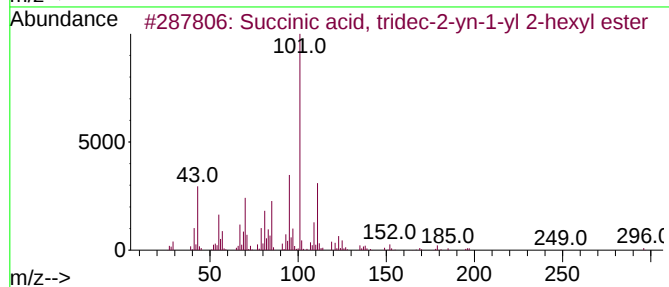
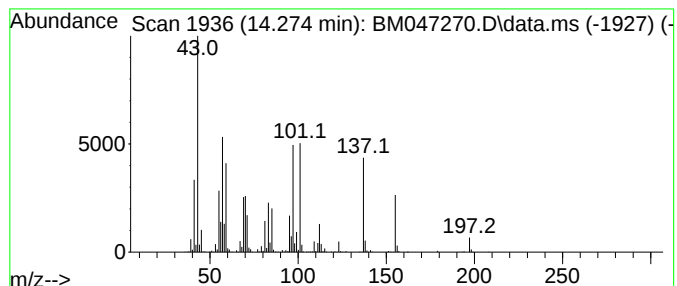
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Peak Number 3 unknown14.274 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	17.23 ng	2011590	Acenaphthene-d10	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, tridec-2-yn-1-yl ...	380	C23H40O4	1000390-69-6	14
2			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
3			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	10
4			Acetoxyacetic acid, 4-tetradecyl...	314	C18H34O4	1000308-80-9	10
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10



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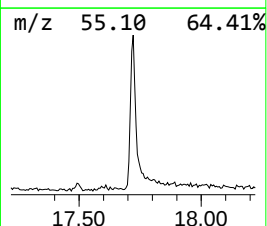
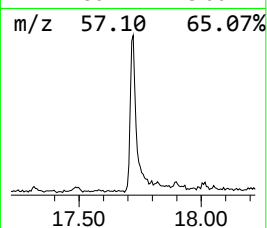
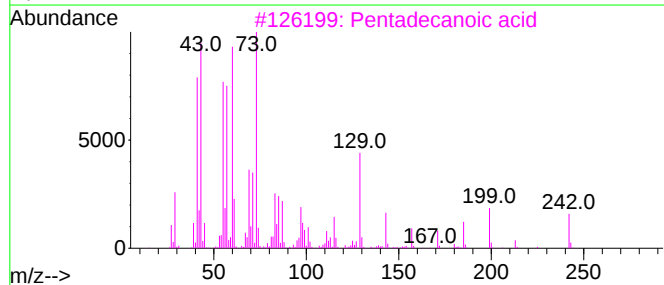
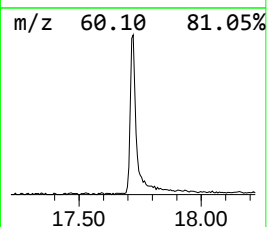
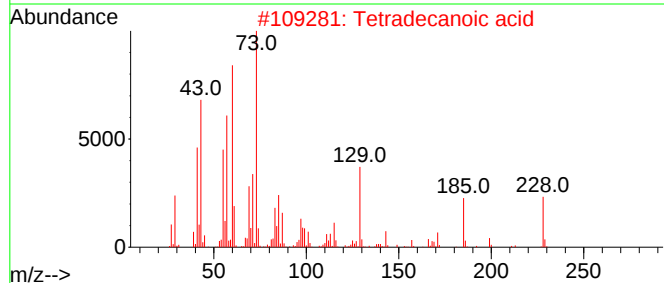
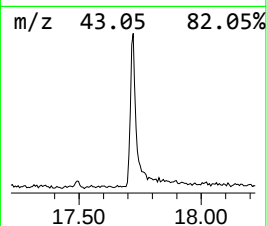
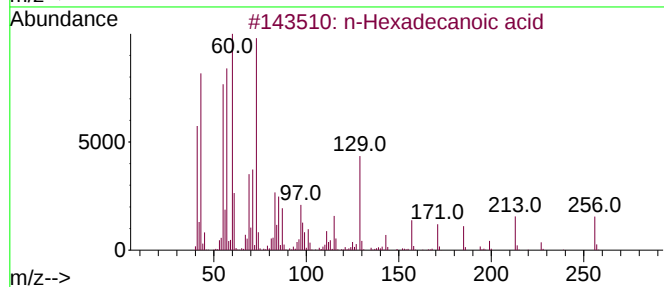
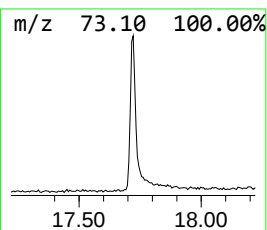
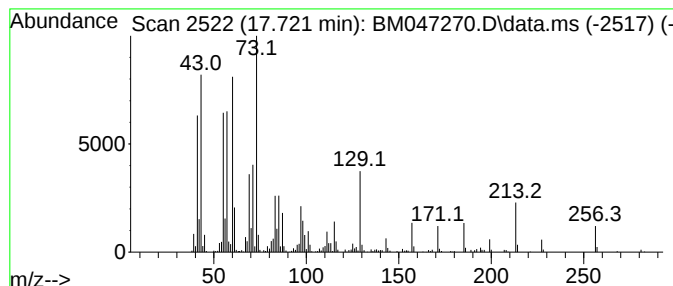
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	3.80 ng	562909	Phenanthrene-d10	16.786

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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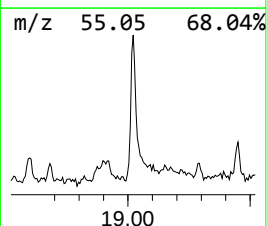
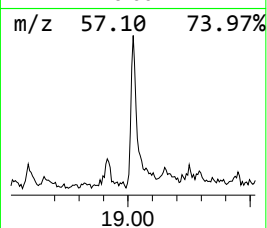
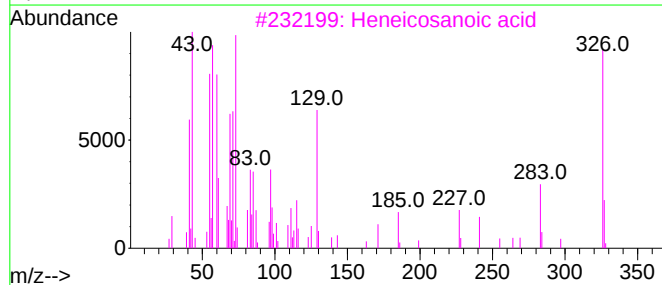
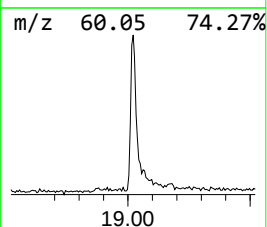
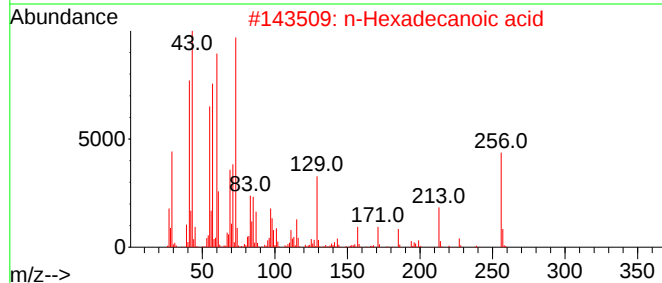
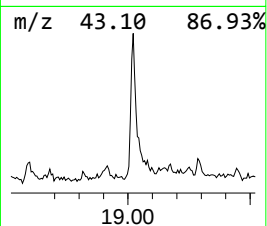
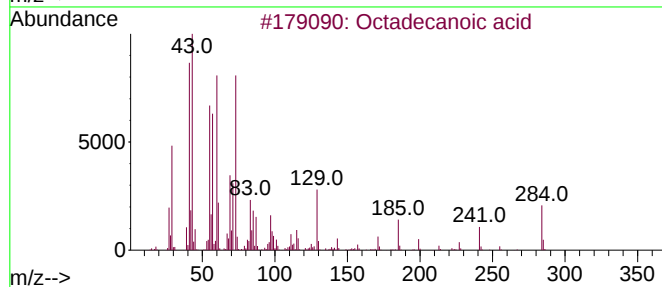
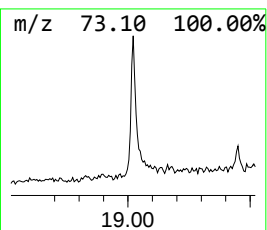
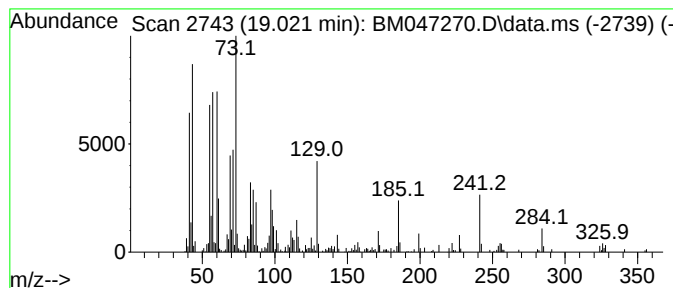
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	2.19 ng	367675	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Heneicosanoic acid	326	C21H42O2	002363-71-5	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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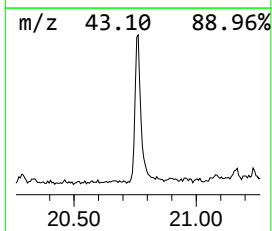
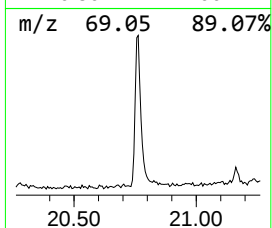
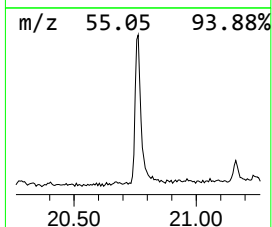
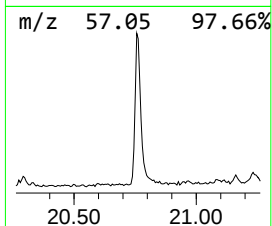
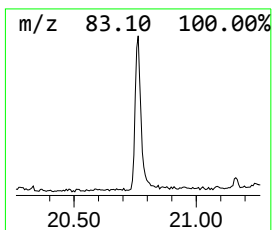
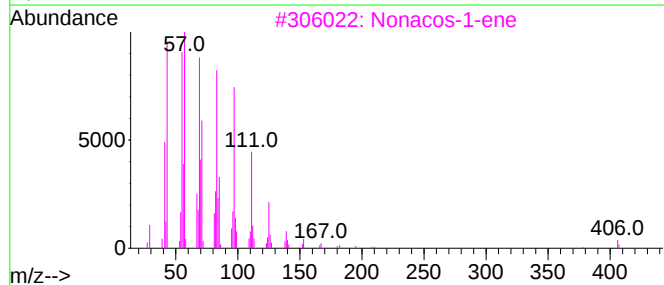
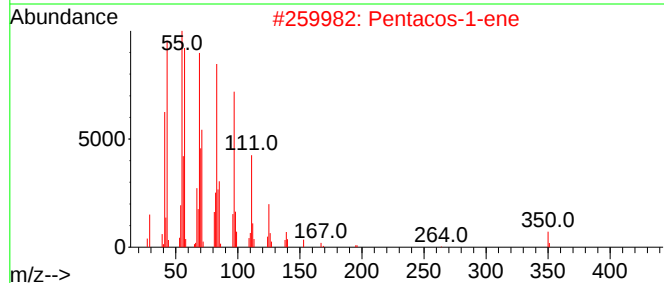
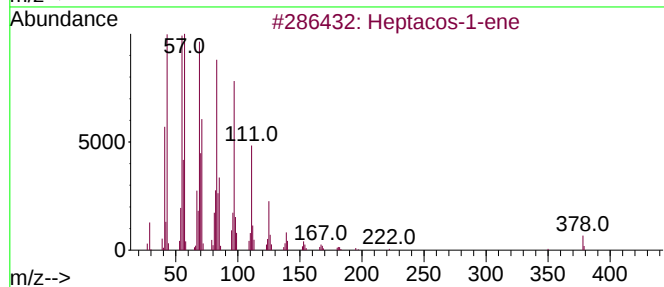
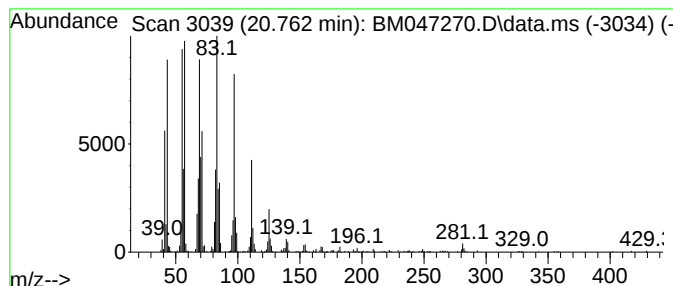
Instrument :
BNA_M
ClientSampleId :
918-J-SD-0.5-1-081524

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 6 Heptacos-1-ene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.762	4.36 ng	731056	Chrysene-d12	21.021	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	94
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Nonacos-1-ene	406	C29H58	018835-35-3	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082024\
Data File : BM047270.D
Acq On : 20 Aug 2024 14:06
Operator : RC/JU
Sample : P3643-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-SD-0.5-1-081524

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.569	3.5	ng	216257	1	7.357	1224460	20.0
1-Phenoxypropan...	10.880	2.1	ng	176122	2	10.116	1662500	20.0
unknown14.274	14.274	17.2	ng	2011590	3	14.015	2335650	20.0
n-Hexadecanoic ...	17.721	3.8	ng	562909	4	16.786	2962140	20.0
Octadecanoic acid	19.021	2.2	ng	367675	5	21.021	3353780	20.0
Heptacos-1-ene	20.762	4.4	ng	731056	5	21.021	3353780	20.0