

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
 Data File : BM047236.D
 Acq On : 16 Aug 2024 15:51
 Operator : RC/JU
 Sample : P3582-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-855-J-SO-1-1.5-081224

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: BM047236.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	61	64	73	rBV	180251	227338	3.75%	0.556%
2	4.575	282	287	295	rVB	176776	243838	4.02%	0.596%
3	5.016	356	362	378	rBV	2804519	3937606	64.88%	9.623%
4	6.575	620	627	639	rBV	2577192	3937630	64.88%	9.623%
5	7.363	755	761	770	rVB	926921	1375328	22.66%	3.361%
6	8.510	948	956	972	rBV	1588828	2569270	42.34%	6.279%
7	9.092	1046	1055	1063	rBV2	49560	82346	1.36%	0.201%
8	10.116	1222	1229	1238	rBV	1031102	1681256	27.70%	4.109%
9	10.881	1351	1359	1369	rBV	132390	290426	4.79%	0.710%
10	12.628	1647	1656	1668	rBV	3369116	4932303	81.27%	12.054%
11	14.022	1886	1893	1904	rBV	1357158	1977092	32.58%	4.832%
12	14.274	1934	1936	1944	rVB3	58723	78207	1.29%	0.191%
13	15.527	2143	2149	2161	rBV	2607607	3668095	60.44%	8.964%
14	16.786	2357	2363	2374	rVB	1491032	2170610	35.77%	5.305%
15	17.721	2517	2522	2538	rBV	564285	1001442	16.50%	2.447%
16	18.257	2609	2613	2623	rBV	53026	91980	1.52%	0.225%
17	18.862	2712	2716	2719	rBV	61112	92562	1.53%	0.226%
18	19.021	2739	2743	2752	rBV	250963	435513	7.18%	1.064%
19	19.174	2765	2769	2772	rBV	103128	116816	1.92%	0.285%
20	19.286	2783	2788	2797	rVB2	63465	134542	2.22%	0.329%
21	19.451	2810	2816	2826	rBV	5059937	6068725	100.00%	14.831%
22	20.233	2946	2949	2954	rBV3	93545	110986	1.83%	0.271%
23	20.768	3036	3040	3049	rBV2	234272	432263	7.12%	1.056%
24	21.021	3078	3083	3088	rBV	1908266	2448038	40.34%	5.983%
25	23.715	3534	3541	3557	rVB	1210242	2814070	46.37%	6.877%

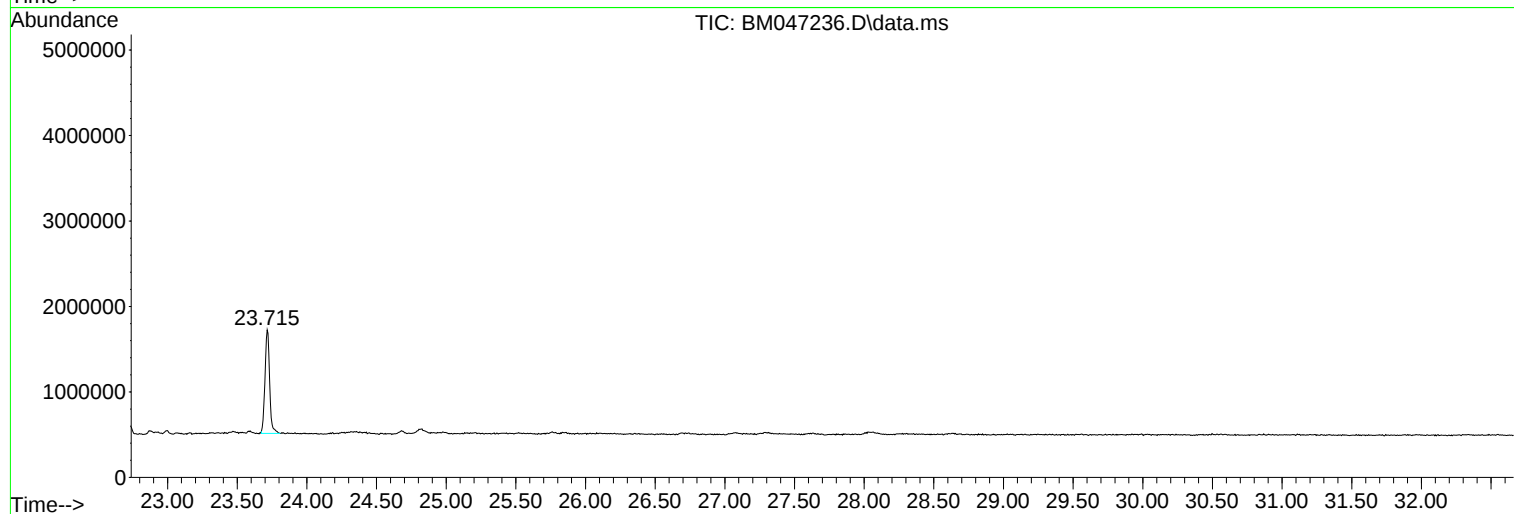
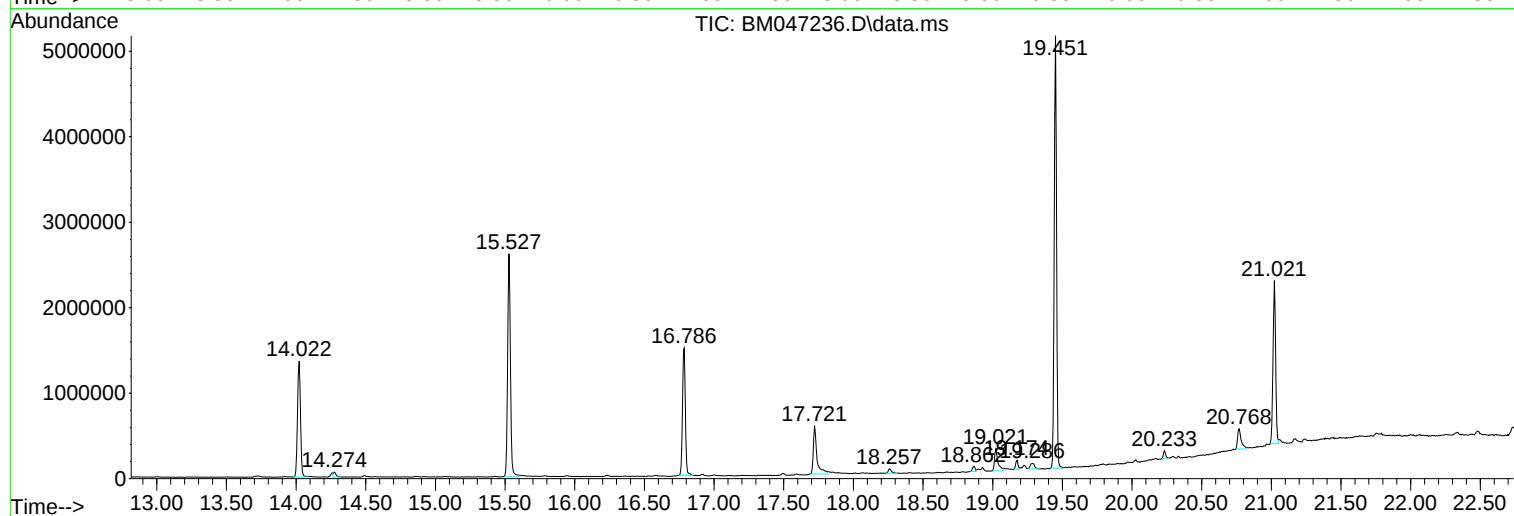
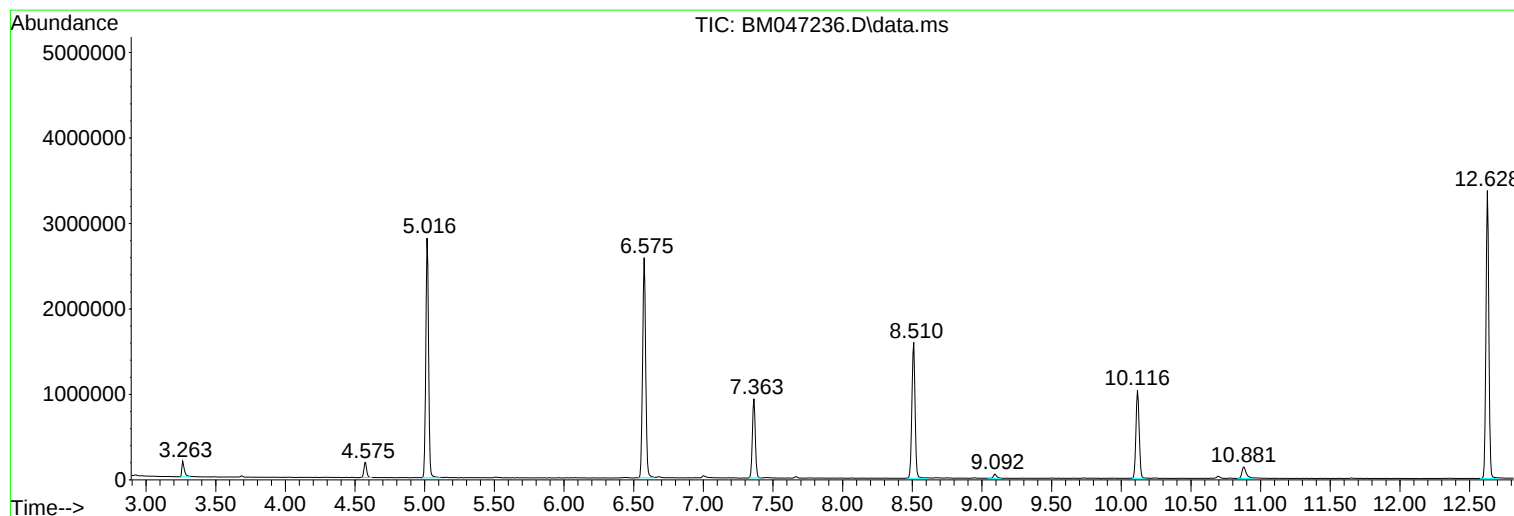
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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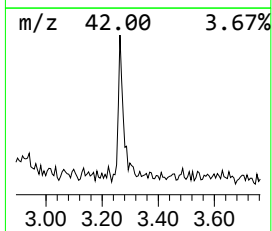
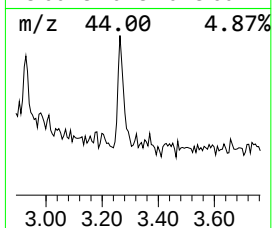
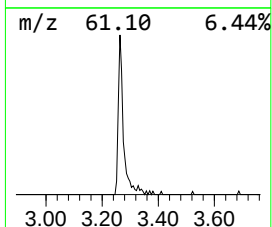
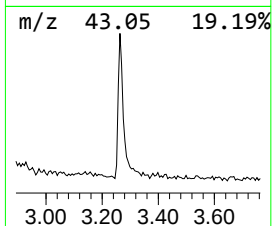
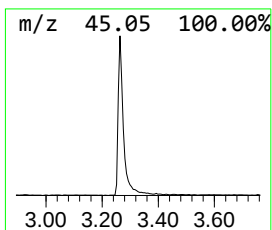
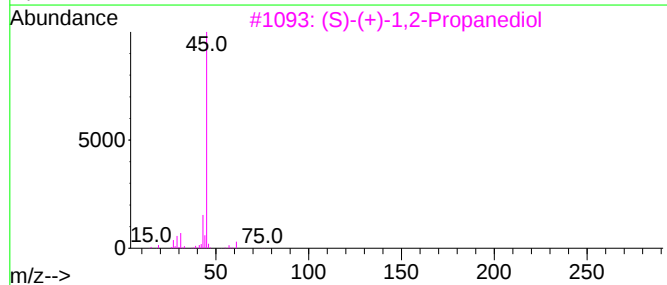
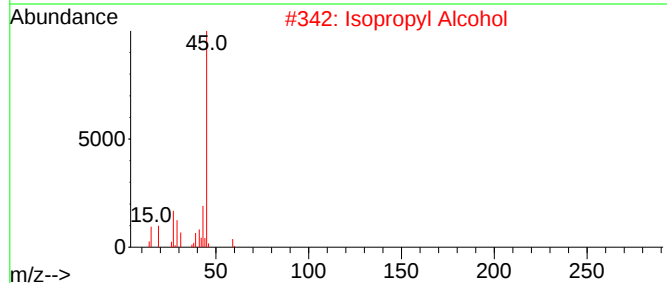
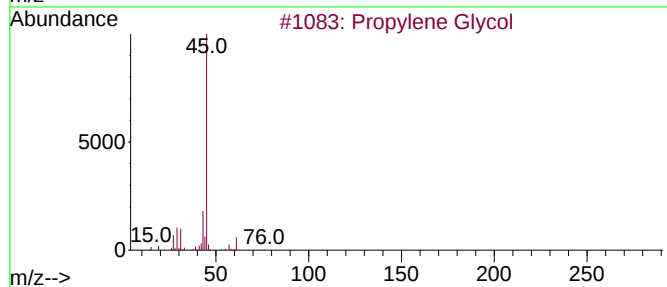
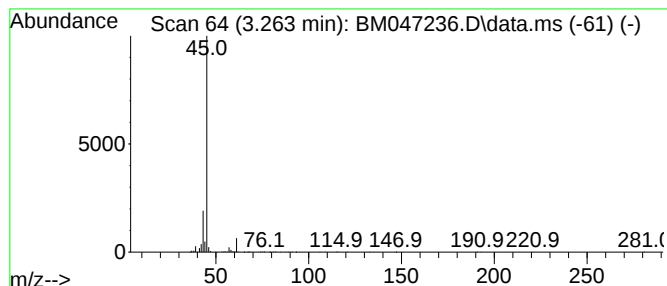
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.263	3.31 ng	227338	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Hexanol	102	C6H14O	000626-93-7	9



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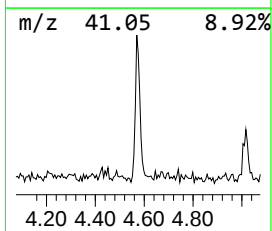
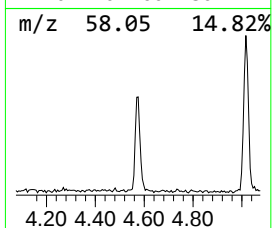
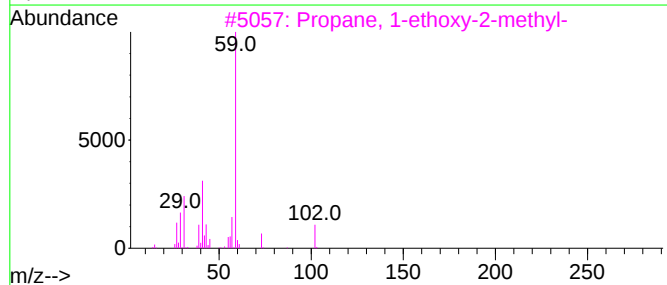
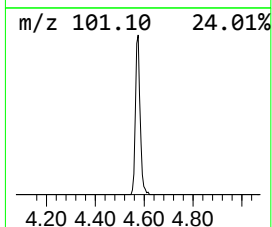
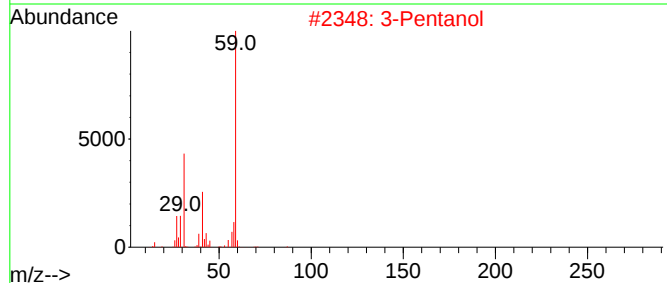
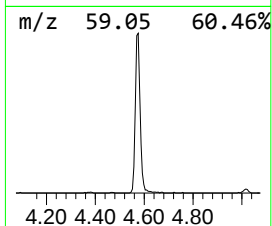
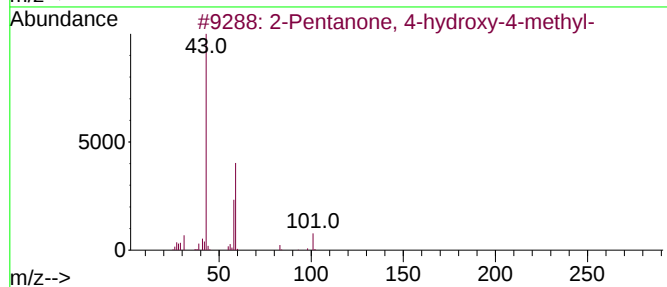
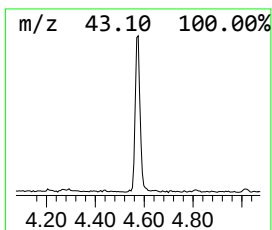
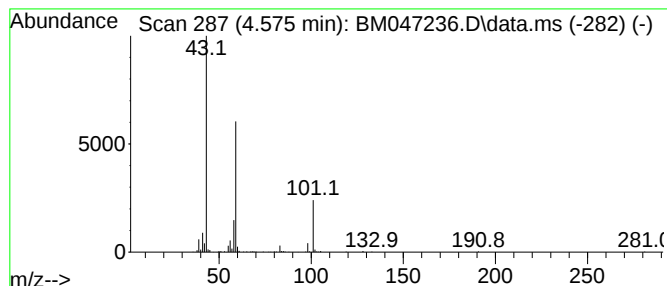
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.575	3.55 ng	243838	1,4-Dichlorobenzene-d4	7.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	3-Pentanol	88	C5H12O	000584-02-1	37		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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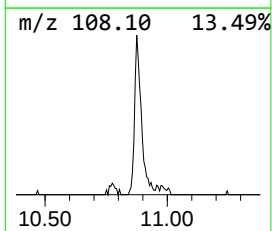
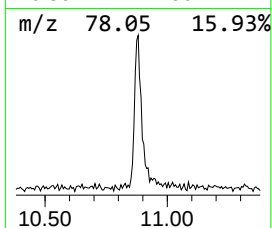
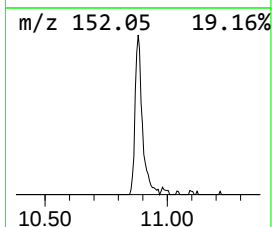
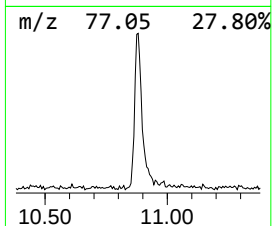
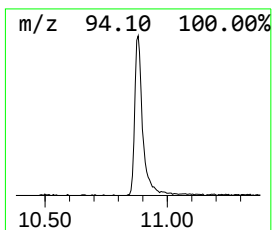
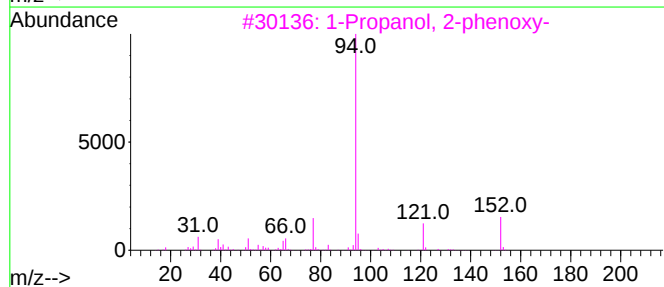
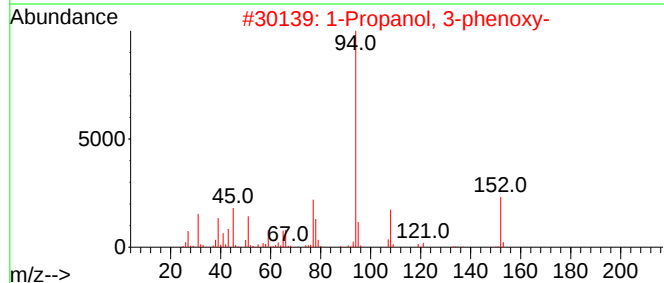
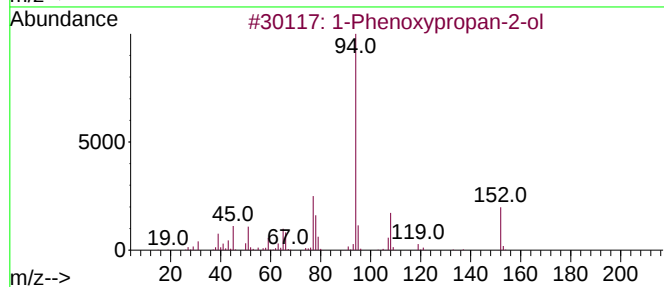
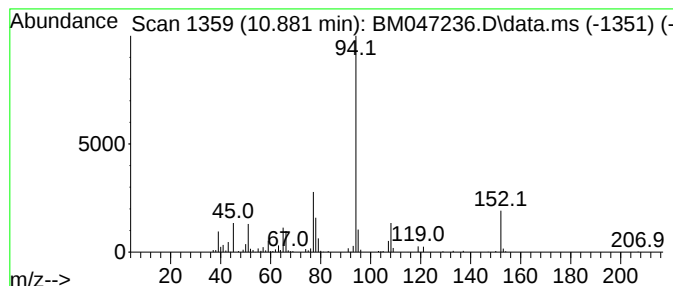
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Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	3.45 ng	290426	Naphthalene-d8	10.116

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	93
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5			3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	53



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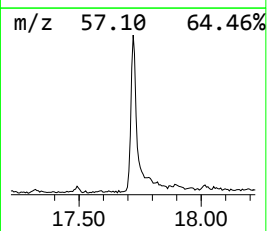
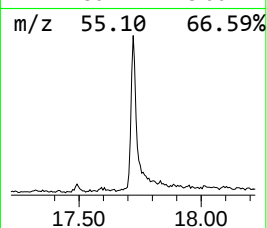
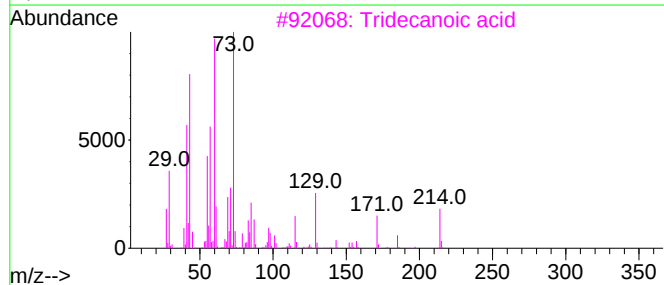
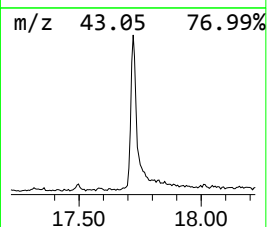
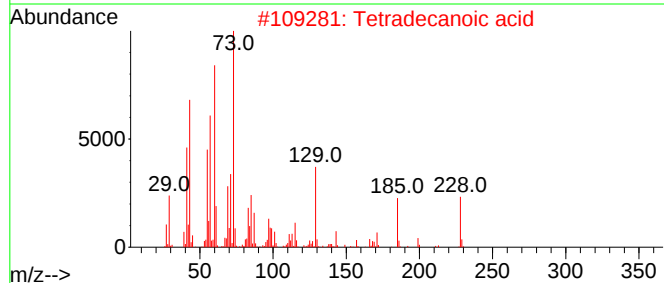
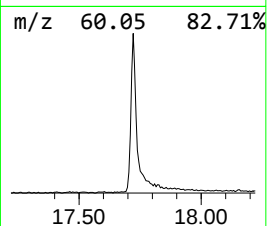
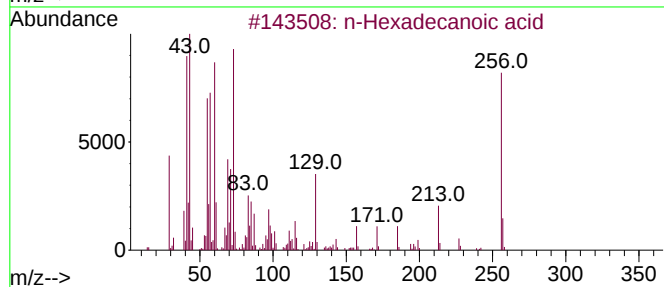
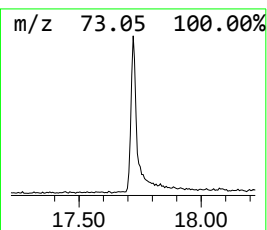
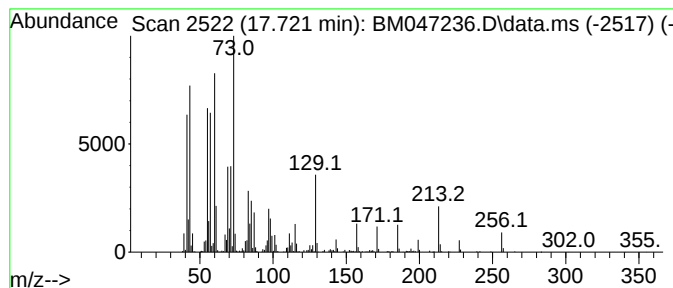
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	9.23 ng	1001440	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			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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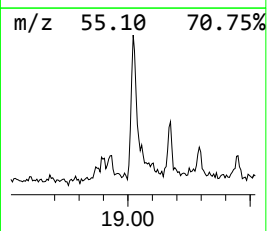
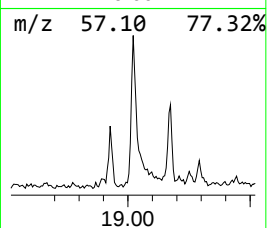
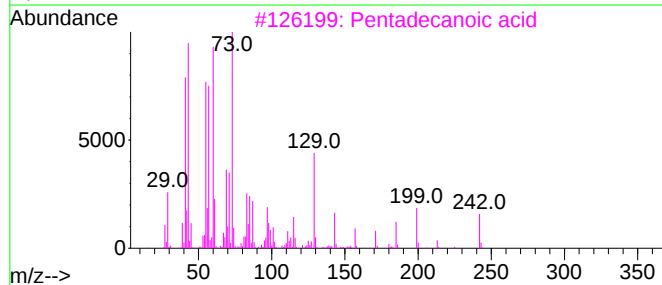
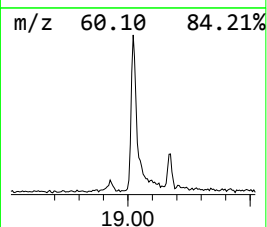
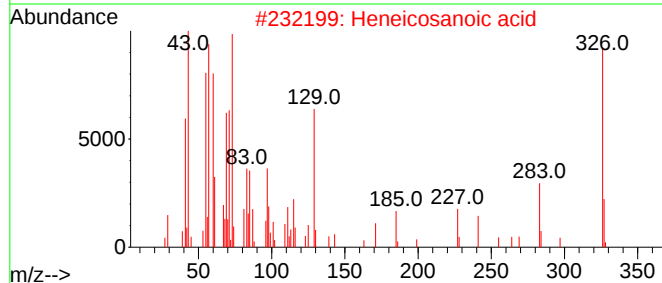
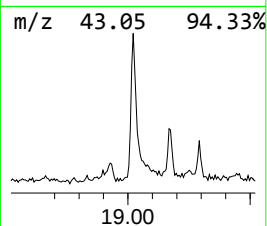
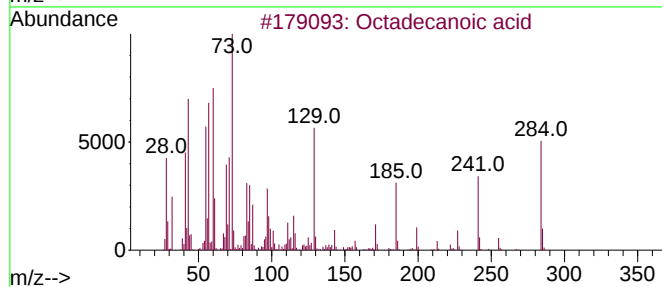
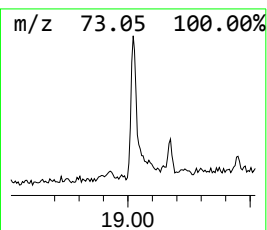
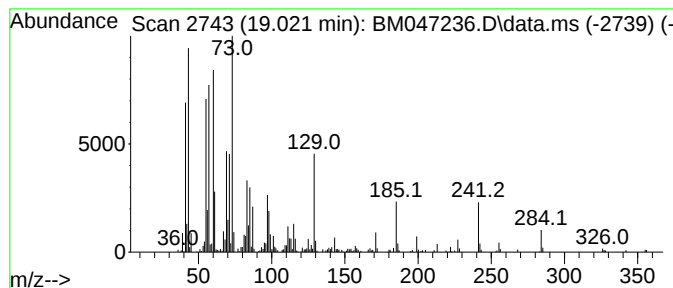
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Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.021	3.56 ng	435513	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Heneicosanoic acid	326	C21H42O2	002363-71-5	97
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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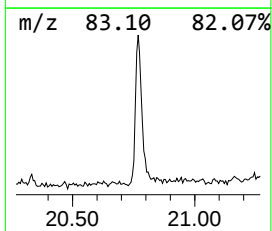
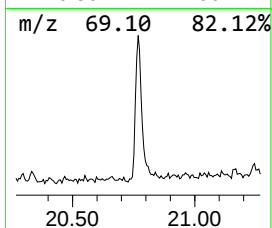
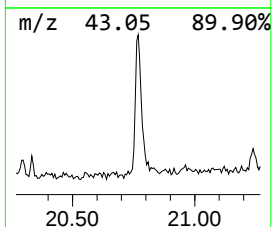
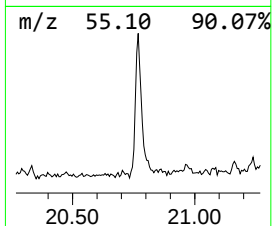
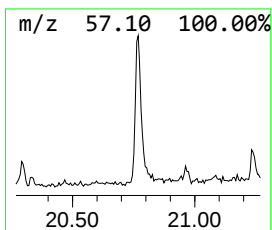
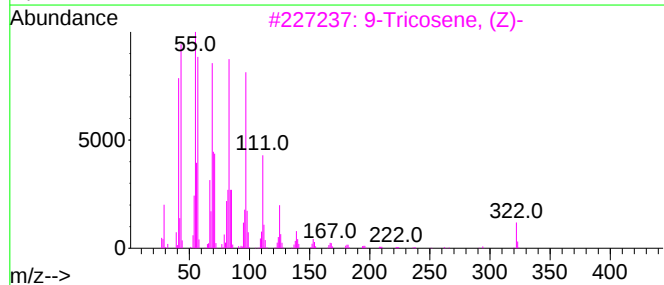
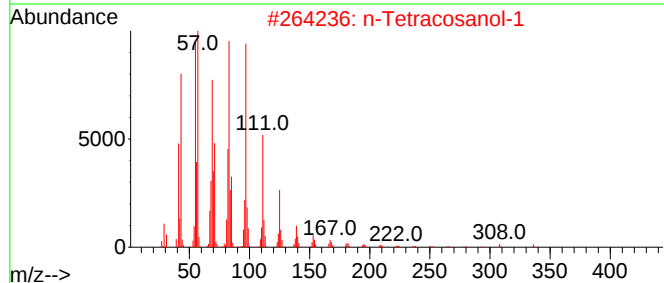
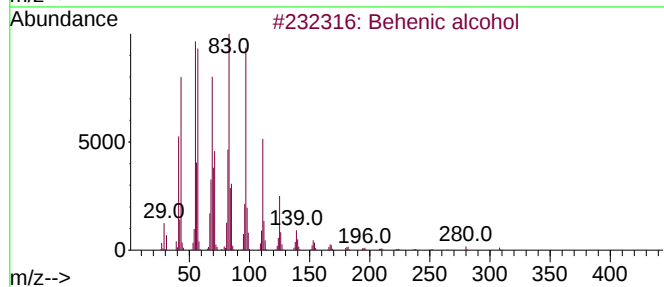
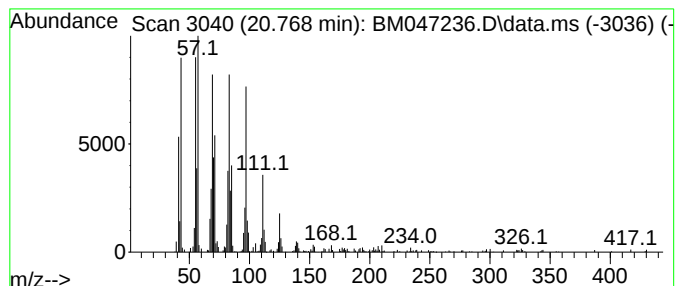
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.768	3.53 ng	432263	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Octacosanol	410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081624\
Data File : BM047236.D
Acq On : 16 Aug 2024 15:51
Operator : RC/JU
Sample : P3582-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-855-J-SO-1-1.5-081224

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.263	3.3	ng	227338	1	7.363	1375330	20.0
2-Pentanone, 4-...	4.575	3.5	ng	243838	1	7.363	1375330	20.0
1-Phenoxypropan...	10.881	3.5	ng	290426	2	10.116	1681260	20.0
n-Hexadecanoic ...	17.721	9.2	ng	1001440	4	16.786	2170610	20.0
Octadecanoic acid	19.021	3.6	ng	435513	5	21.021	2448040	20.0
Behenic alcohol	20.768	3.5	ng	432263	5	21.021	2448040	20.0