

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
 Data File : BM047314.D
 Acq On : 22 Aug 2024 13:11
 Operator : RC/JU
 Sample : P3671-14
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-912-J-SO-0.5-1-081924

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: BM047314.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	79	rVB	109407	176496	3.31%	0.413%
2	4.563	279	285	292	rBV	154882	217924	4.08%	0.509%
3	5.010	355	361	374	rBV	2250551	3303272	61.87%	7.721%
4	6.569	619	626	645	rBV	2085989	3447622	64.57%	8.058%
5	7.351	752	759	768	rBV	923562	1419790	26.59%	3.318%
6	7.651	804	810	817	rVB	210387	318442	5.96%	0.744%
7	8.498	941	954	970	rBV	1429445	2407527	45.09%	5.627%
8	9.087	1049	1054	1063	rBV3	42611	88739	1.66%	0.207%
9	10.104	1220	1227	1239	rBV	1120706	1892660	35.45%	4.424%
10	10.875	1350	1358	1376	rBV	84389	232032	4.35%	0.542%
11	12.616	1647	1654	1671	rBV	2673008	4232219	79.27%	9.892%
12	14.010	1885	1891	1909	rBV	1741167	2625539	49.17%	6.137%
13	14.269	1926	1935	1941	rBV5	72880	153740	2.88%	0.359%
14	15.521	2142	2148	2160	rBV	2543115	3856805	72.23%	9.015%
15	16.774	2355	2361	2372	rVB	2078780	3138350	58.78%	7.335%
16	16.986	2392	2397	2402	rBV5	69757	142236	2.66%	0.332%
17	17.545	2486	2492	2509	rVB3	87702	252894	4.74%	0.591%
18	17.680	2510	2515	2517	rBV	138470	197072	3.69%	0.461%
19	17.710	2517	2520	2534	rVV	330706	598511	11.21%	1.399%
20	17.821	2536	2539	2547	rVB5	42524	68450	1.28%	0.160%
21	19.015	2738	2742	2749	rBV	108772	171062	3.20%	0.400%
22	19.445	2809	2815	2827	rBV	4301887	5339305	100.00%	12.480%
23	20.756	3033	3038	3050	rBV	529805	977015	18.30%	2.284%
24	21.015	3077	3082	3090	rBV	2503694	3509698	65.73%	8.203%
25	21.774	3207	3211	3222	rVB	321482	659956	12.36%	1.543%
26	23.709	3532	3540	3553	rVB	1465471	3356758	62.87%	7.846%

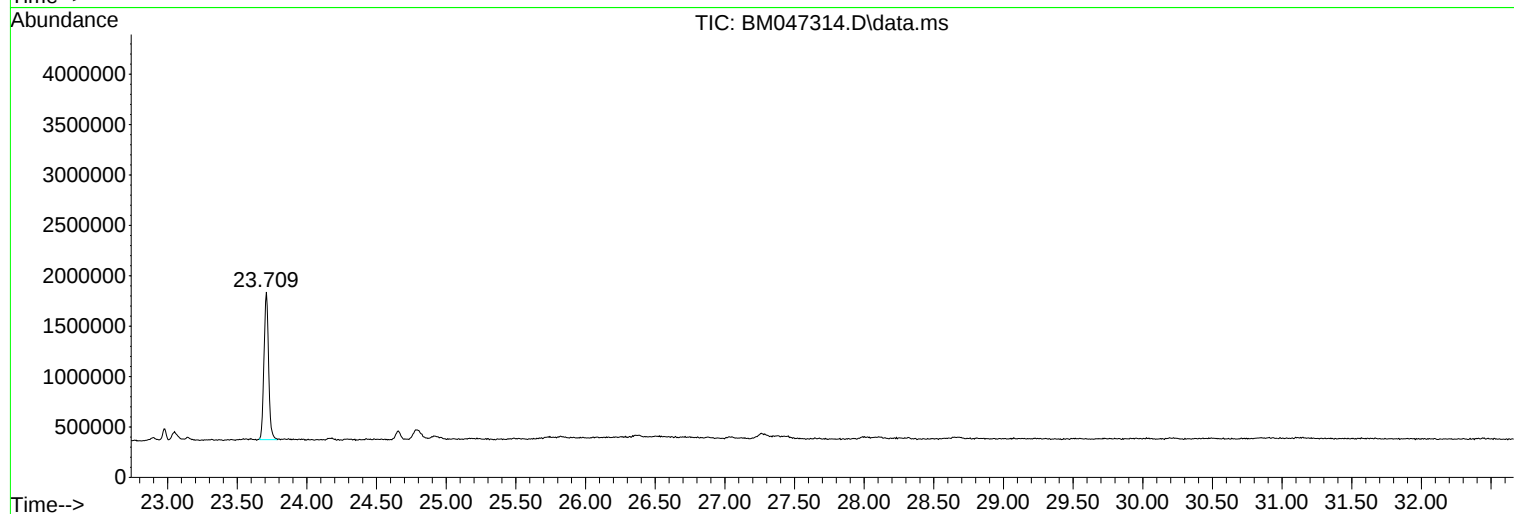
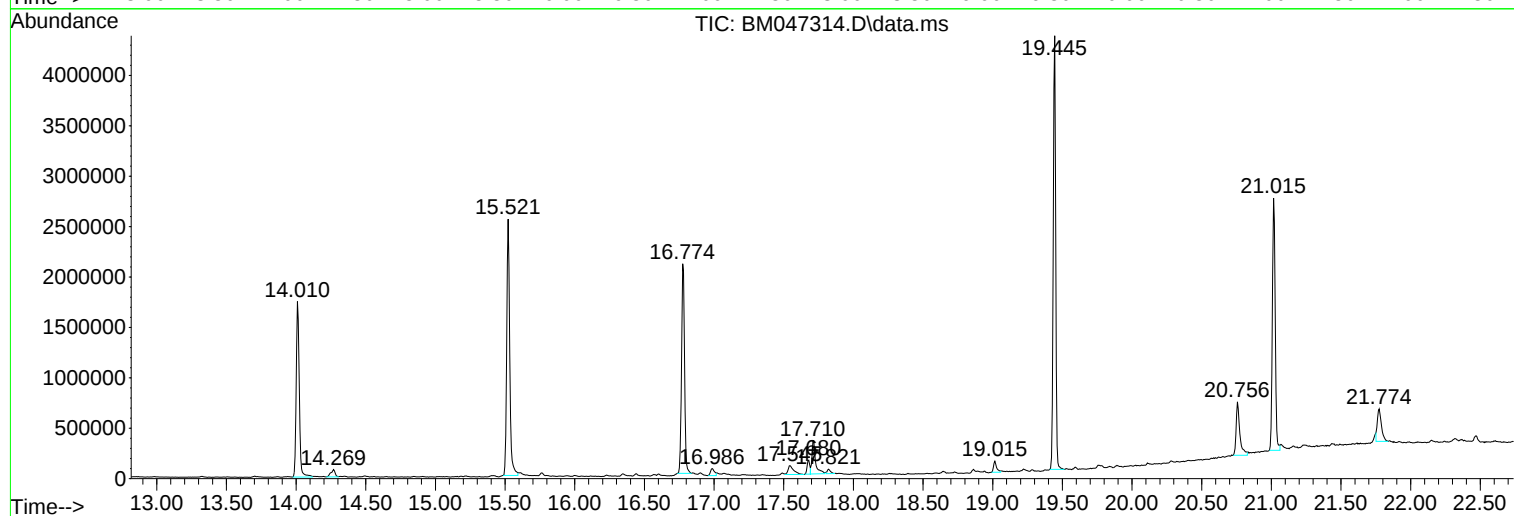
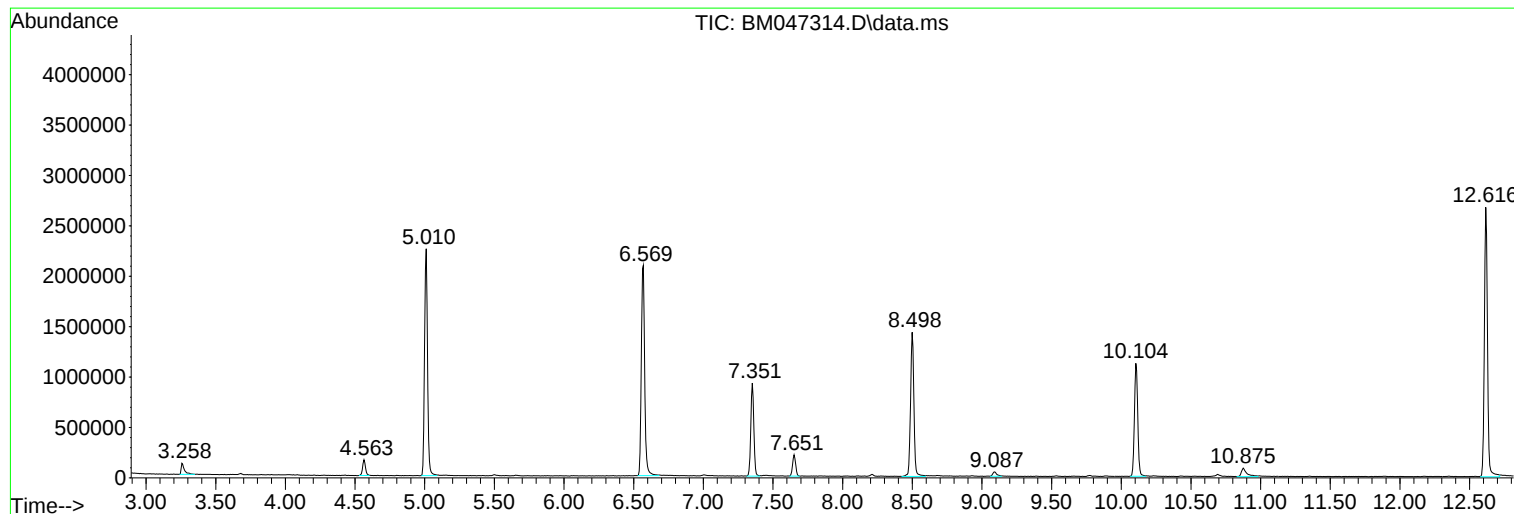
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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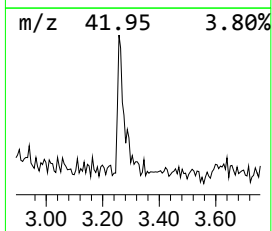
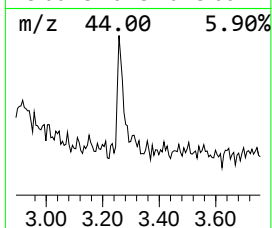
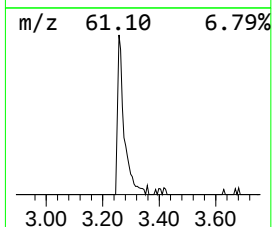
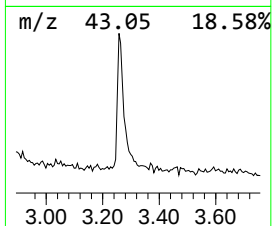
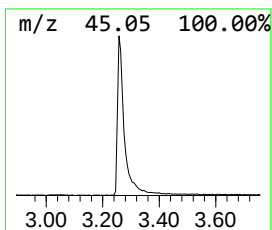
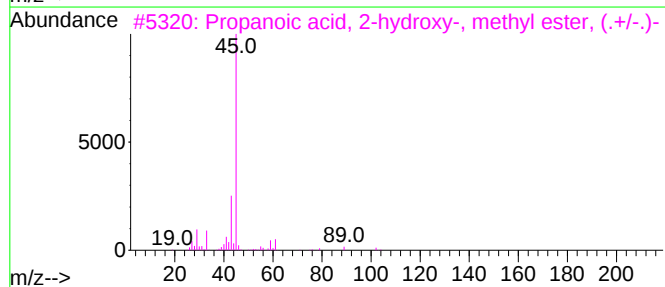
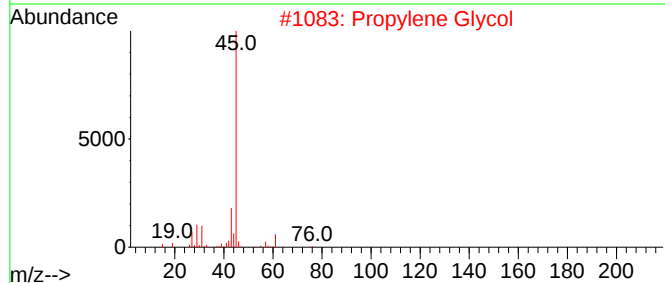
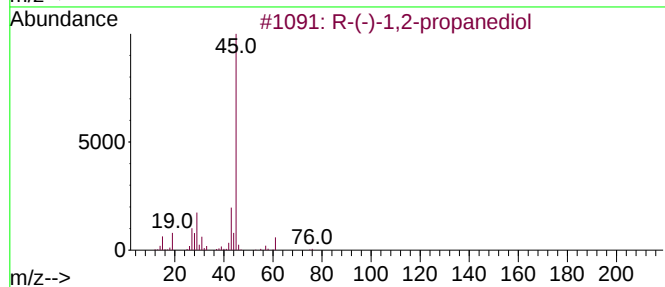
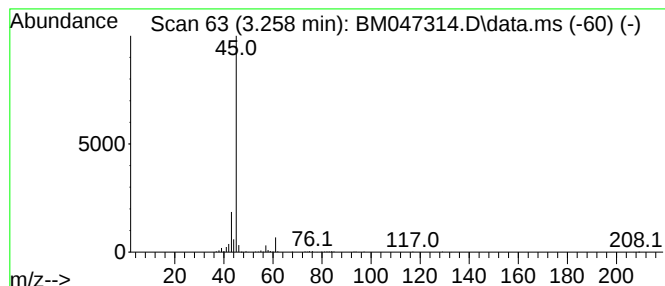
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	2.49 ng	176496	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2			Propylene Glycol	76	C3H8O2	000057-55-6	78
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9
5			2-Heptanol	116	C7H16O	000543-49-7	9



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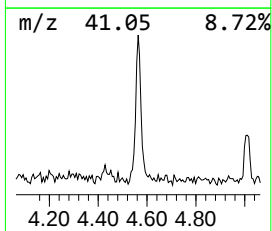
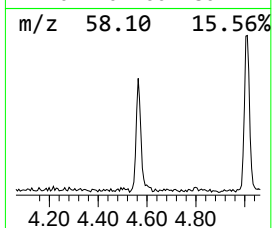
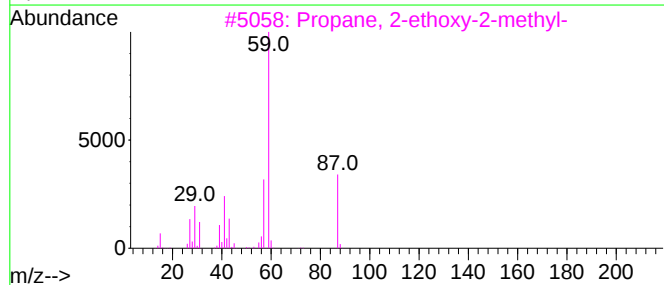
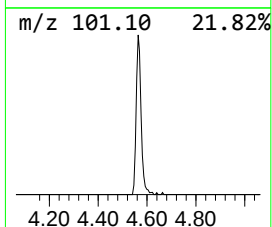
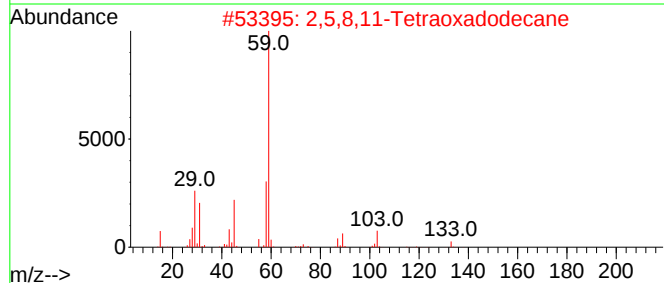
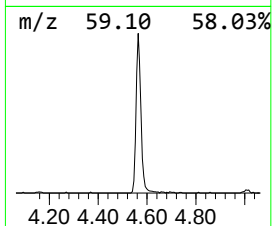
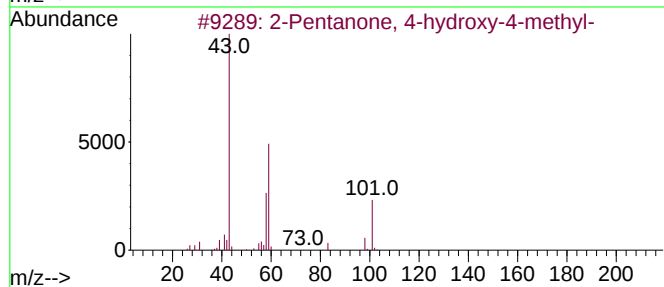
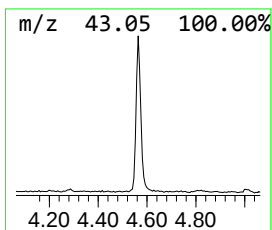
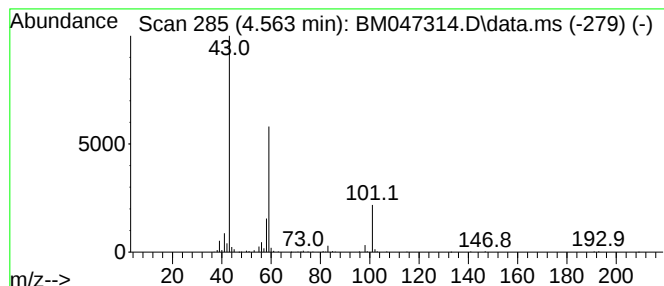
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	3.07 ng	217924	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	47
2		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23
3		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
4		Hexanamide	115	C6H13NO	000628-02-4	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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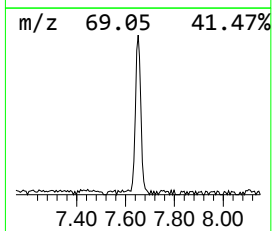
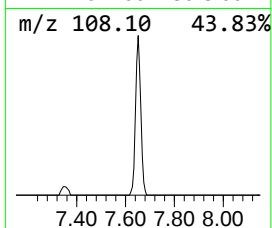
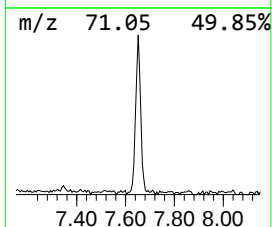
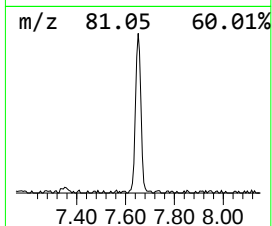
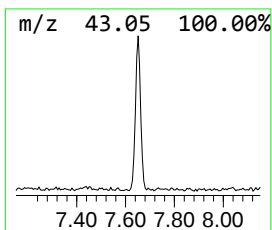
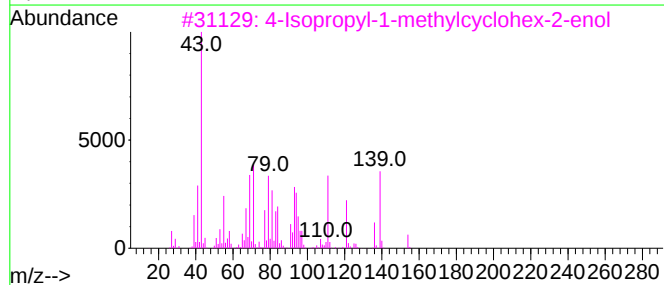
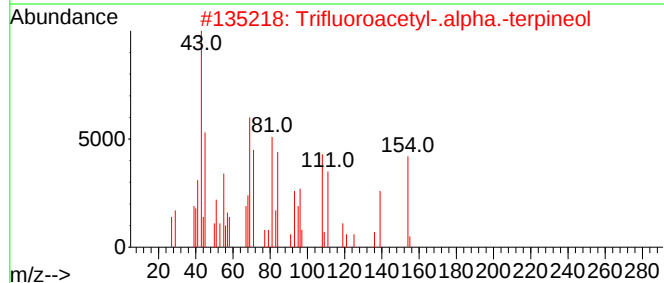
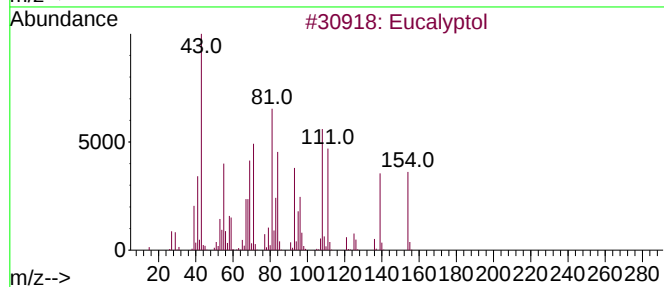
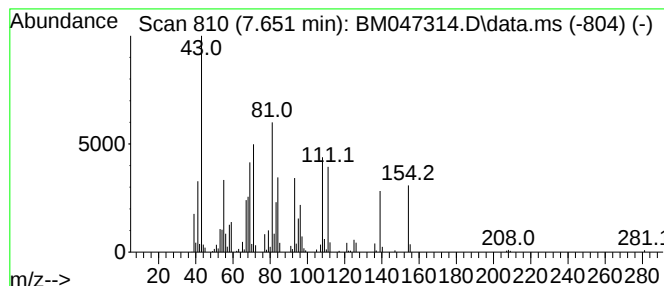
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.651	4.49 ng	318442	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	47
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	32
4			2-Cyano-1-(thiiran-2-yl)ethyl ac...	171	C7H9N0S5	1000477-78-4	27
5			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27



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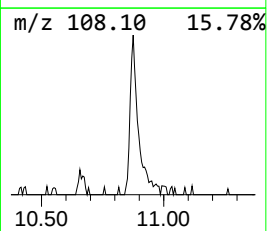
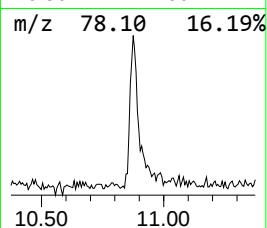
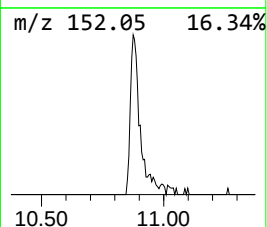
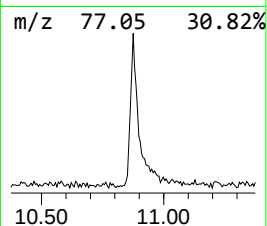
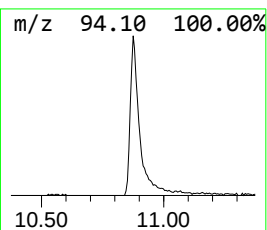
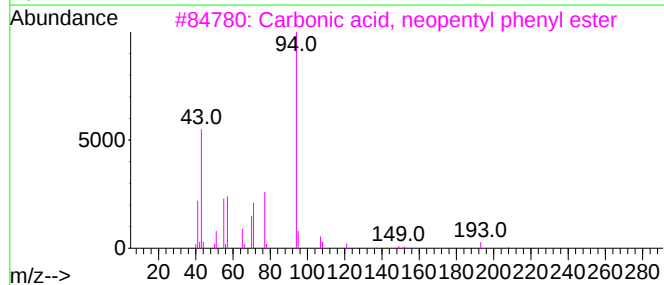
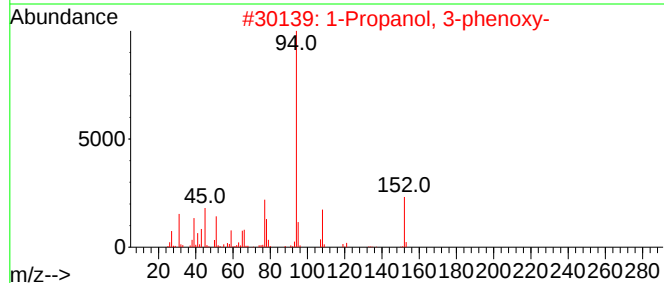
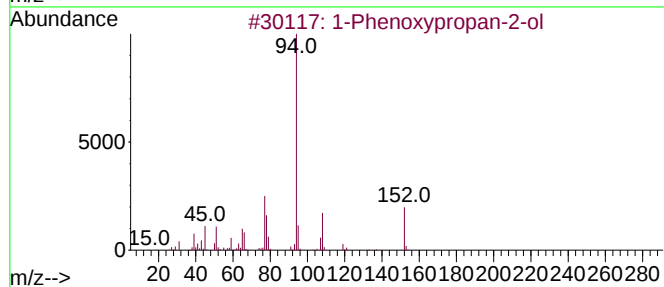
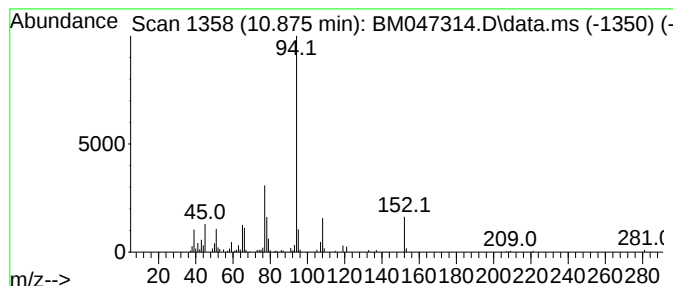
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.45 ng	232032	Naphthalene-d8	10.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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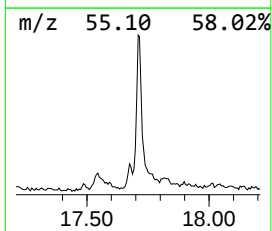
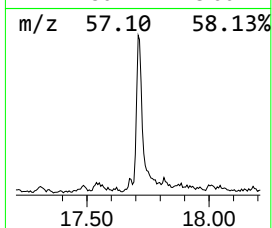
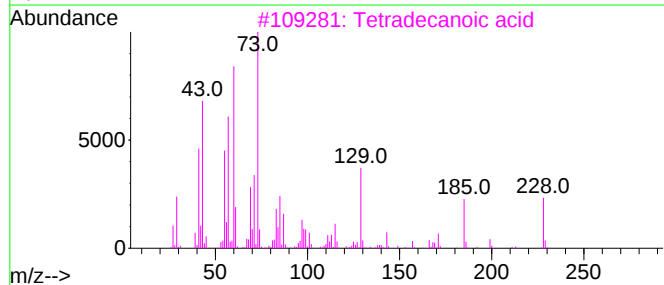
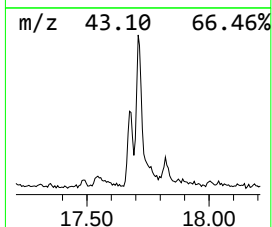
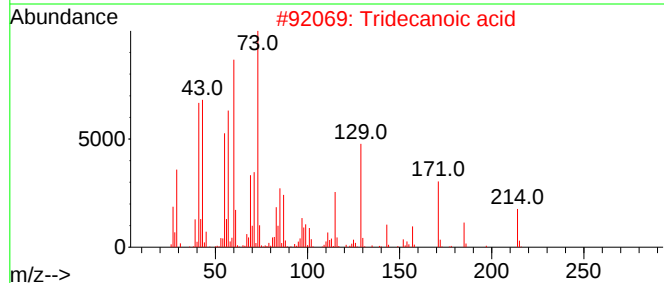
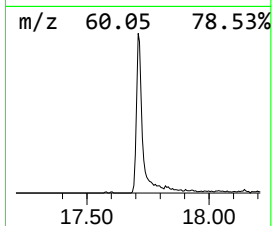
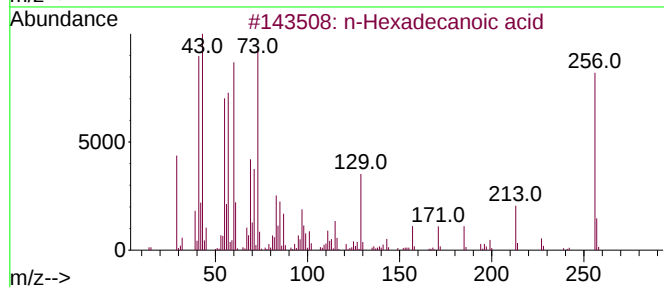
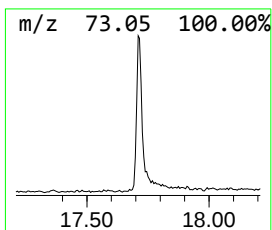
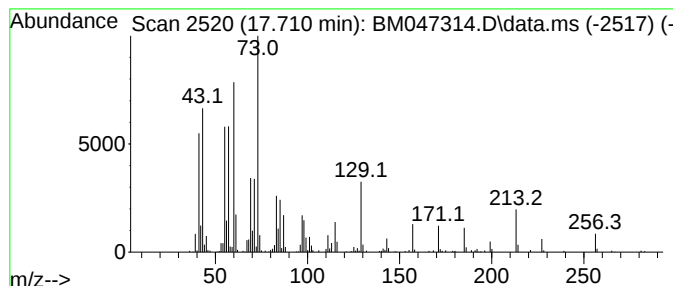
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.710	3.81 ng	598511	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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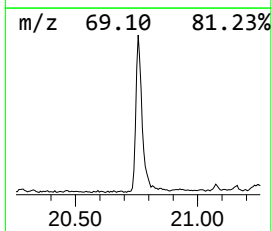
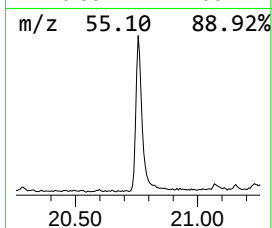
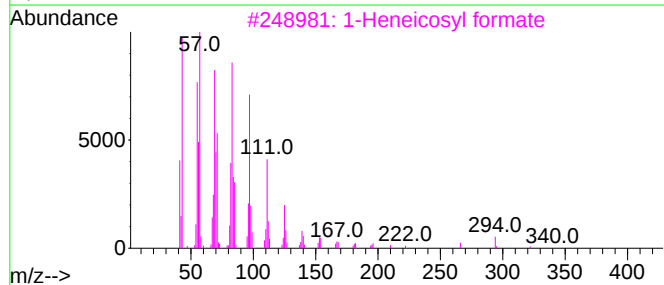
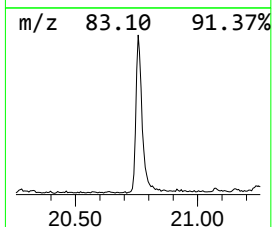
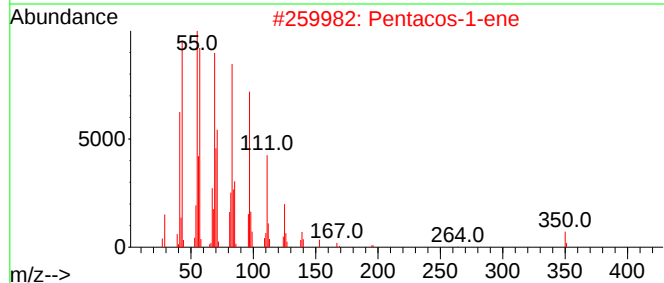
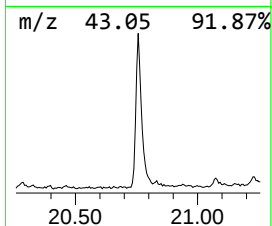
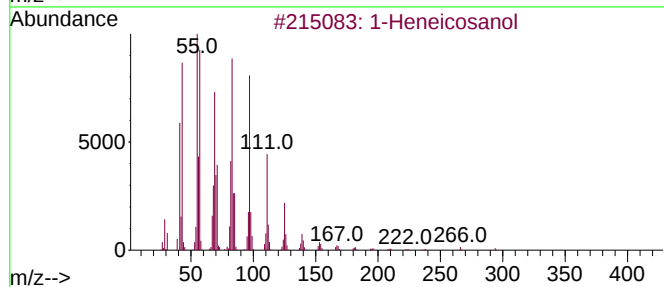
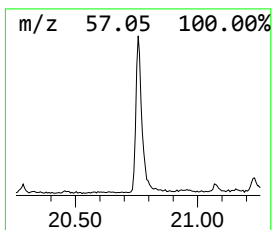
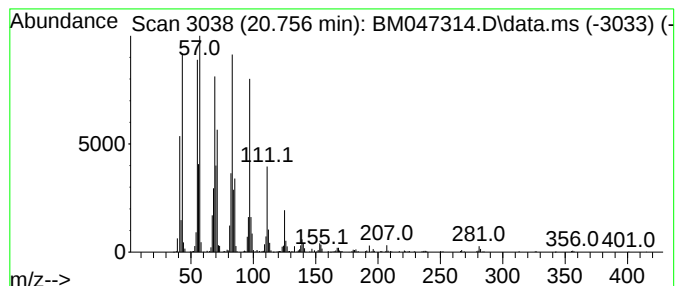
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	5.57 ng	977015	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Heptacos-1-ene	378	C27H54	015306-27-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047314.D
Acq On : 22 Aug 2024 13:11
Operator : RC/JU
Sample : P3671-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-912-J-SO-0.5-1-081924

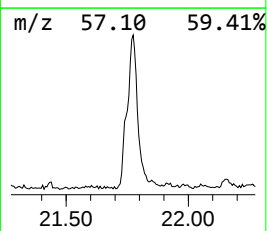
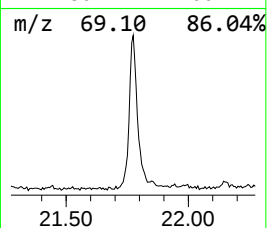
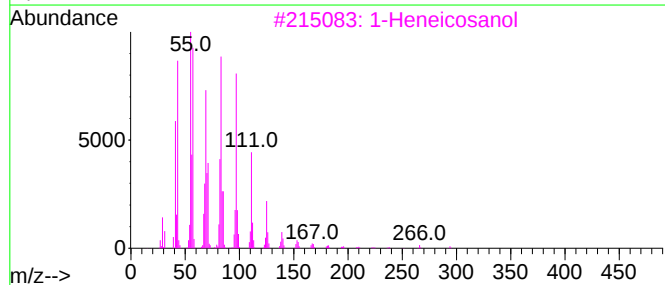
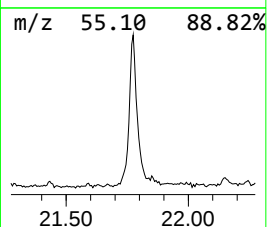
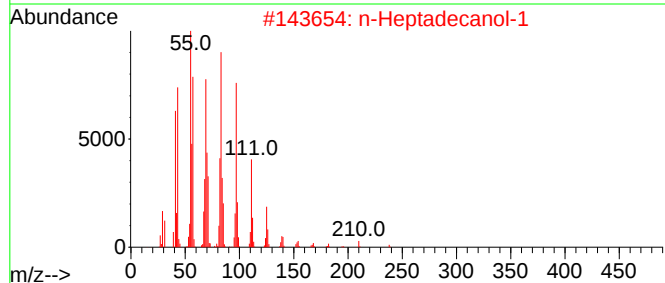
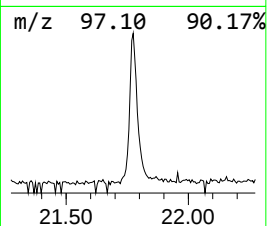
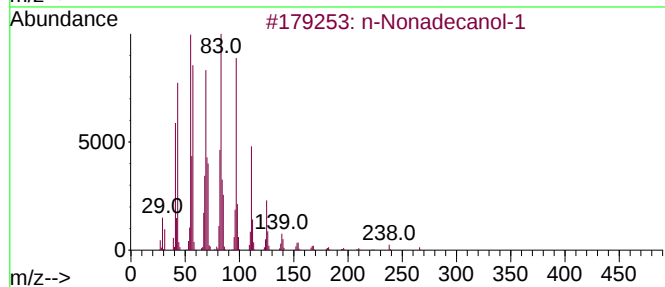
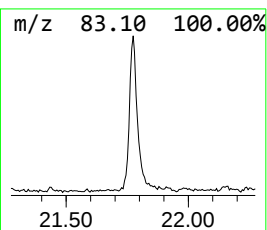
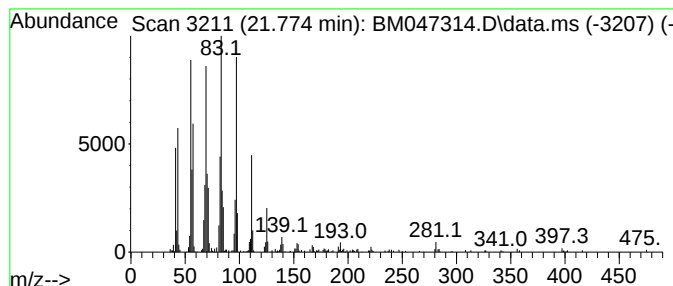
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.774	3.76 ng	659956	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	81
4			1-Octadecanol, methyl ether	284	C19H40O	1000406-29-3	81
5			Behenic alcohol	326	C22H46O	000661-19-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047314.D
Acq On : 22 Aug 2024 13:11
Operator : RC/JU
Sample : P3671-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-912-J-SO-0.5-1-081924

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
R-(-)-1,2-propa...	3.258	2.5	ng	176496	1	7.351	1419790	20.0
2-Pentanone, 4-...	4.563	3.1	ng	217924	1	7.351	1419790	20.0
Eucalyptol	7.651	4.5	ng	318442	1	7.351	1419790	20.0
1-Phenoxypropan...	10.875	2.5	ng	232032	2	10.104	1892660	20.0
n-Hexadecanoic ...	17.710	3.8	ng	598511	4	16.774	3138350	20.0
1-Heneicosanol	20.756	5.6	ng	977015	5	21.015	3509700	20.0
n-Nonadecanol-1	21.774	3.8	ng	659956	5	21.015	3509700	20.0