

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
 Data File : BM047316.D
 Acq On : 22 Aug 2024 14:31
 Operator : RC/JU
 Sample : P3671-13
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-912-J-SO-0-0.5-081924

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: BM047316.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	76	rVB	140740	205849	4.34%	0.429%
2	4.563	278	285	294	rBV	192202	273972	5.78%	0.570%
3	5.010	355	361	379	rBV	2571830	3753493	79.17%	7.814%
4	6.569	619	626	639	rBV	2420366	3994528	84.25%	8.316%
5	7.351	752	759	769	rBV	949984	1440388	30.38%	2.999%
6	7.651	804	810	815	rBV	153967	228798	4.83%	0.476%
7	8.498	941	954	968	rBV	1691616	2813516	59.34%	5.857%
8	9.087	1049	1054	1066	rBV	58672	106440	2.24%	0.222%
9	10.104	1217	1227	1244	rBV	1208591	1987497	41.92%	4.138%
10	10.687	1318	1326	1336	rBV5	26470	56686	1.20%	0.118%
11	10.875	1351	1358	1370	rBV	106944	258898	5.46%	0.539%
12	12.616	1647	1654	1673	rBV	2798609	4276610	90.20%	8.903%
13	14.010	1884	1891	1903	rBV	1786310	2690641	56.75%	5.601%
14	14.245	1927	1931	1932	rBV	49108	53954	1.14%	0.112%
15	14.269	1932	1935	1941	rVB3	70876	101555	2.14%	0.211%
16	15.521	2142	2148	2160	rBV	2730057	4120989	86.92%	8.579%
17	16.774	2355	2361	2367	rBV	2302479	3216697	67.85%	6.696%
18	16.904	2380	2383	2391	rVB4	32071	55238	1.17%	0.115%
19	16.986	2391	2397	2403	rBV7	53955	112120	2.36%	0.233%
20	17.545	2487	2492	2497	rBV6	46856	96217	2.03%	0.200%
21	17.674	2507	2514	2517	rBV3	162145	258095	5.44%	0.537%
22	17.715	2517	2521	2536	rVV	735066	1158604	24.44%	2.412%
23	17.821	2536	2539	2548	rVB5	44069	97660	2.06%	0.203%
24	18.857	2710	2715	2719	rBV	171103	259328	5.47%	0.540%
25	19.009	2737	2741	2755	rBV	270859	473620	9.99%	0.986%
26	19.221	2770	2777	2781	rBV	132775	200104	4.22%	0.417%
27	19.274	2781	2786	2795	rVB	122971	228714	4.82%	0.476%
28	19.439	2809	2814	2826	rVB	3643280	4741231	100.00%	9.870%
29	19.757	2865	2868	2872	rBV3	52329	89031	1.88%	0.185%
30	20.751	3033	3037	3048	rBV	703759	1231836	25.98%	2.564%
31	21.015	3076	3082	3087	rBV	2620361	3578343	75.47%	7.449%
32	21.768	3203	3210	3222	rVB2	530666	1247362	26.31%	2.597%
33	22.974	3411	3415	3421	rVB	299066	504368	10.64%	1.050%
34	23.709	3532	3540	3556	rVB	1507855	3455105	72.87%	7.193%
35	24.656	3696	3701	3709	rVB2	283546	668227	14.09%	1.391%

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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

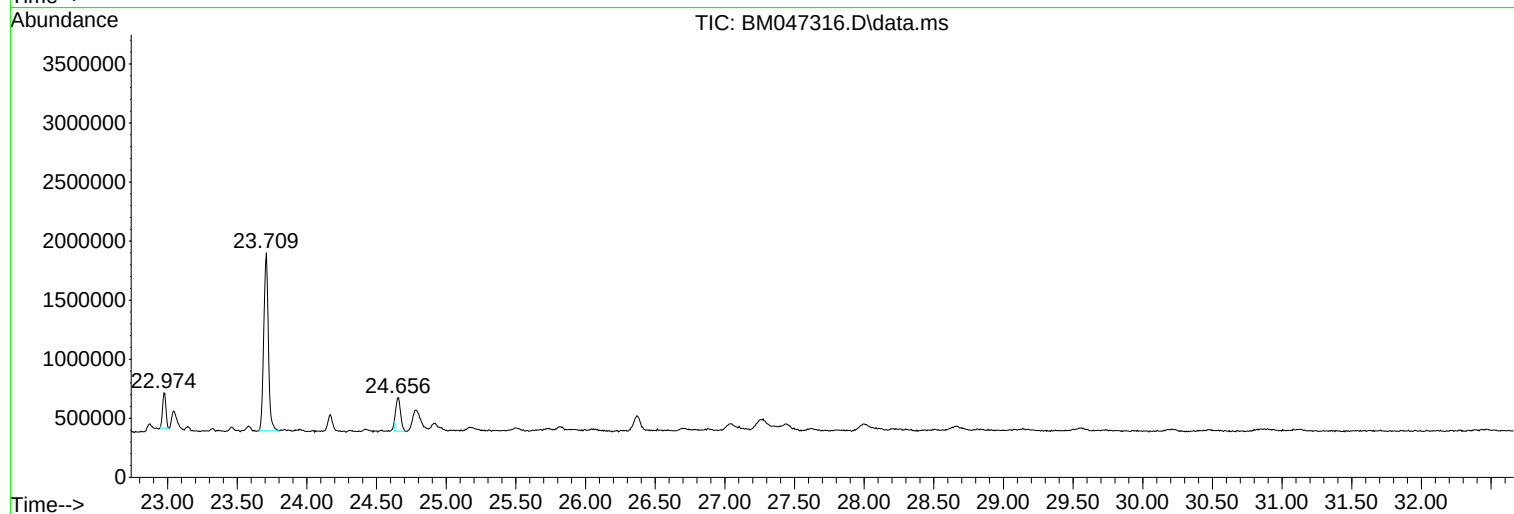
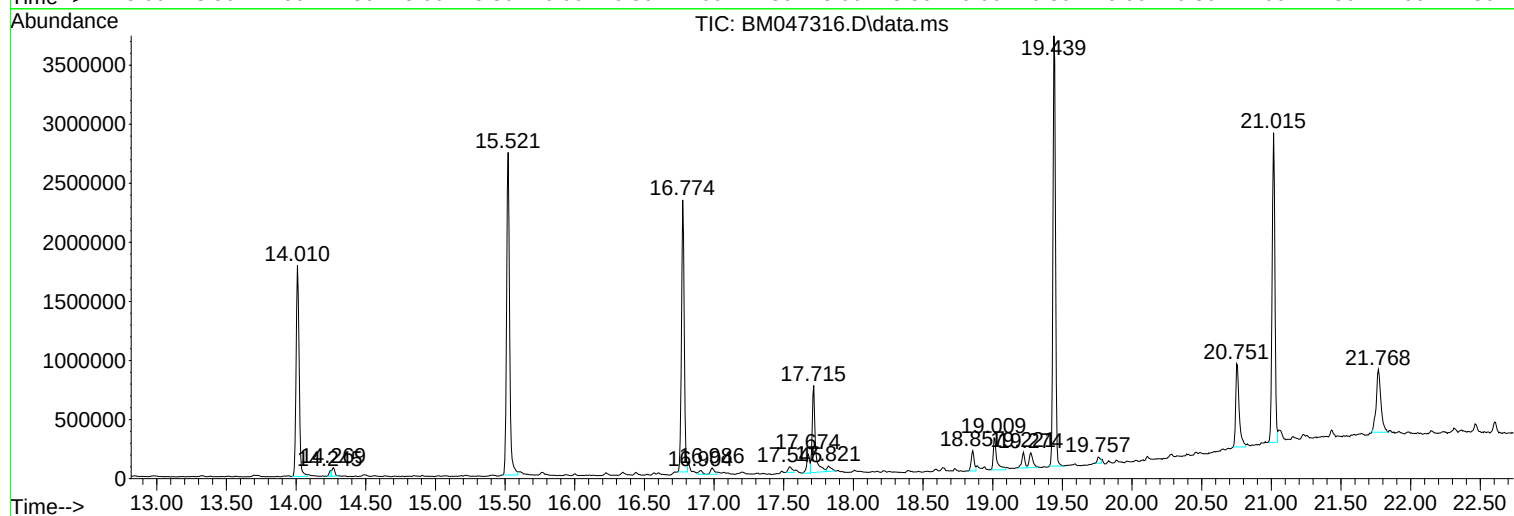
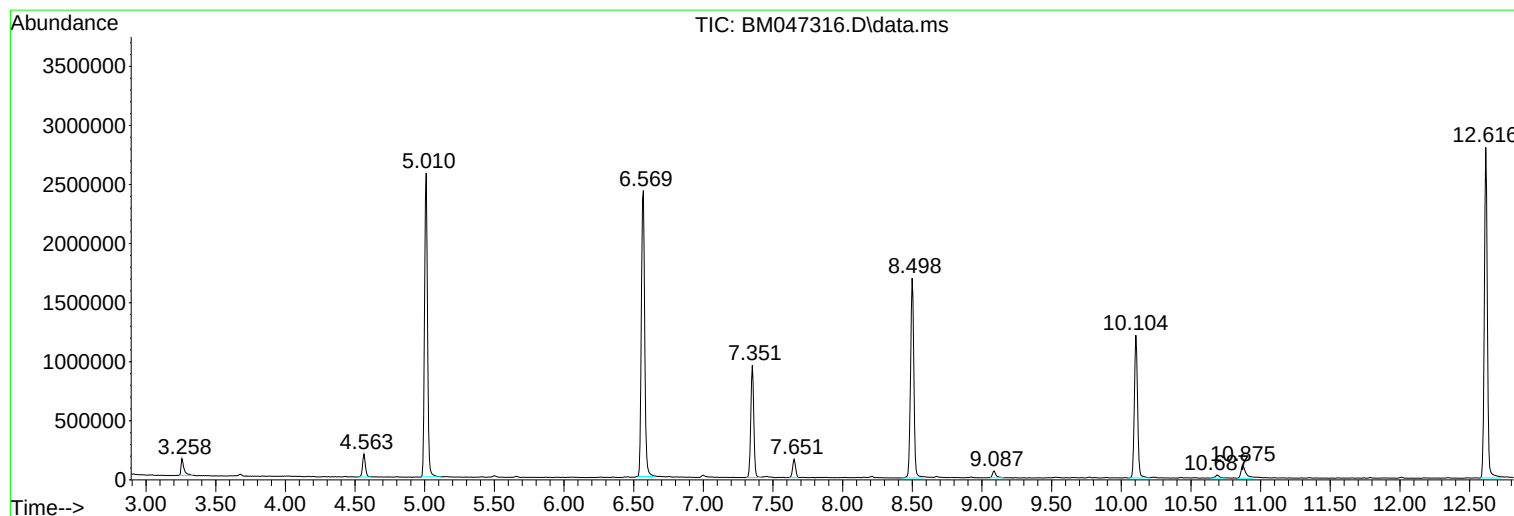
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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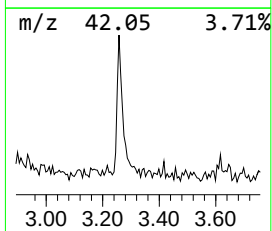
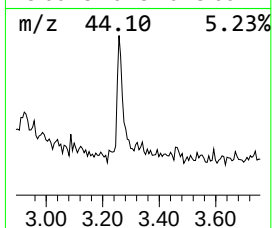
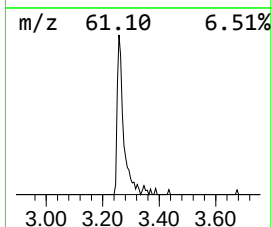
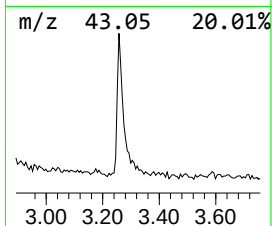
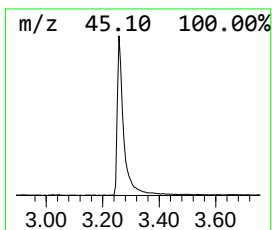
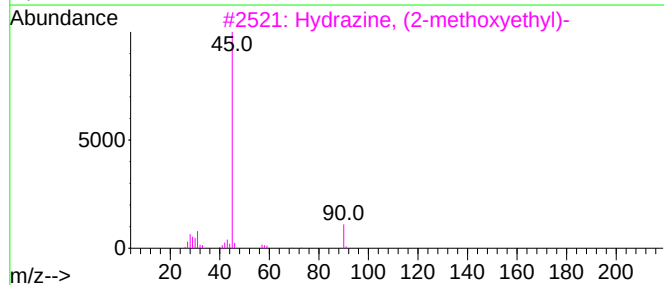
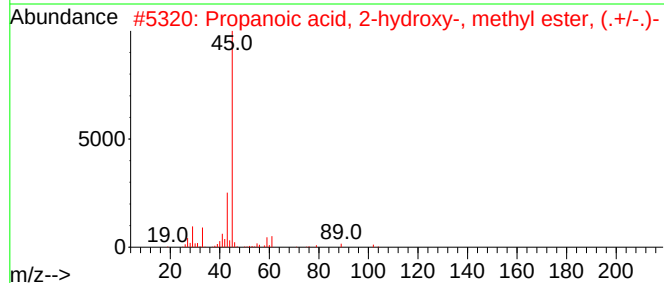
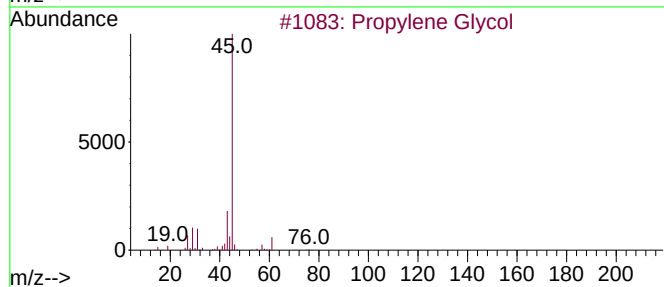
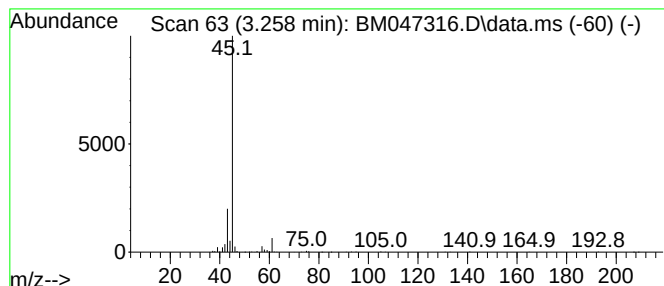
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	2.86 ng	205849	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3			Hydrazine, (2-methoxyethyl)-	90	C3H10N2O	003044-15-3	40
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	40
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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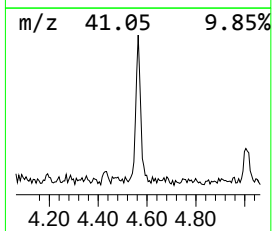
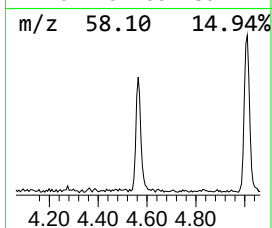
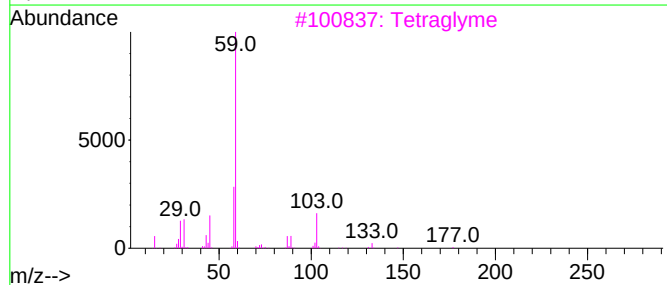
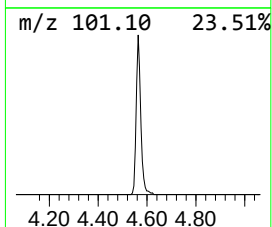
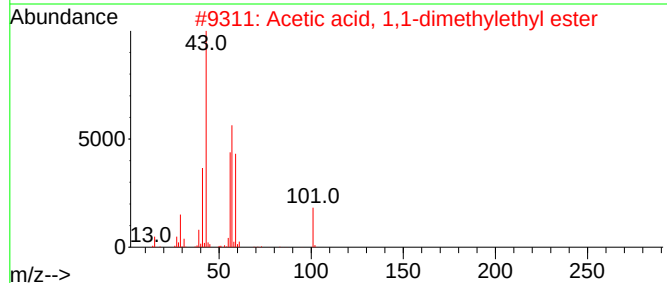
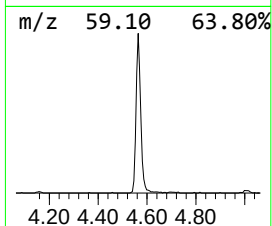
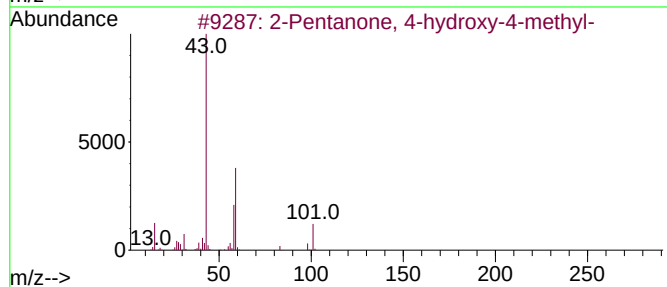
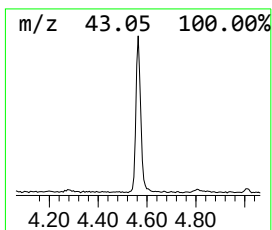
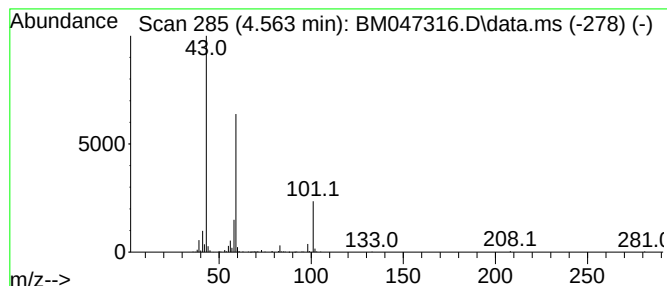
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	3.80 ng	273972	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	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Tetraglyme	222	C10H22O5	000143-24-8	32
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			3-Hexanol	102	C6H14O	000623-37-0	25



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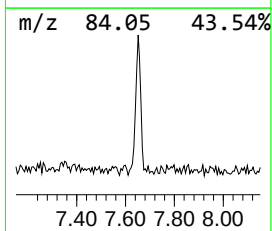
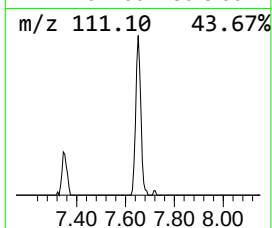
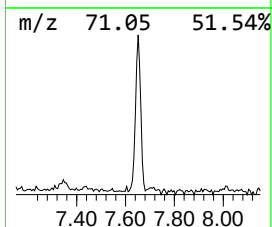
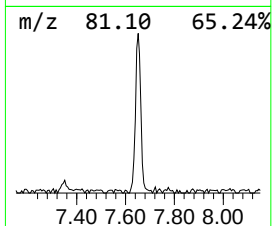
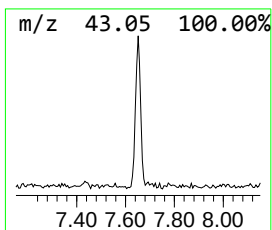
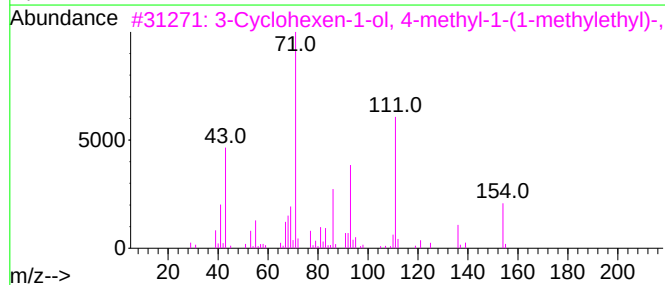
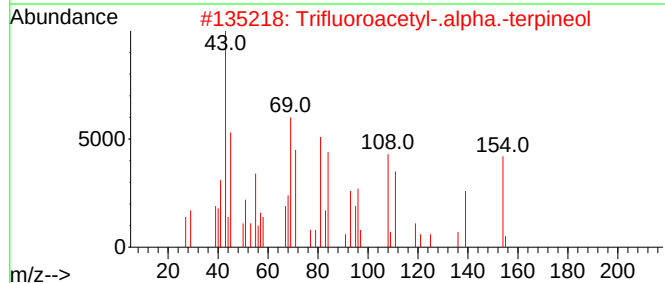
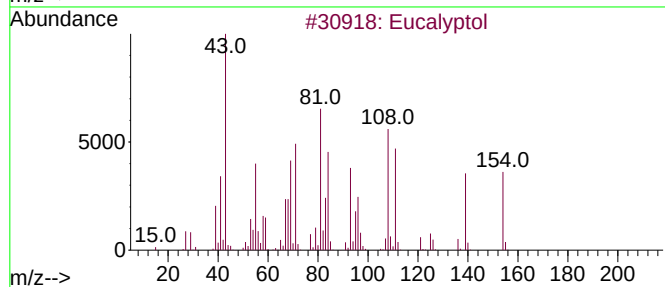
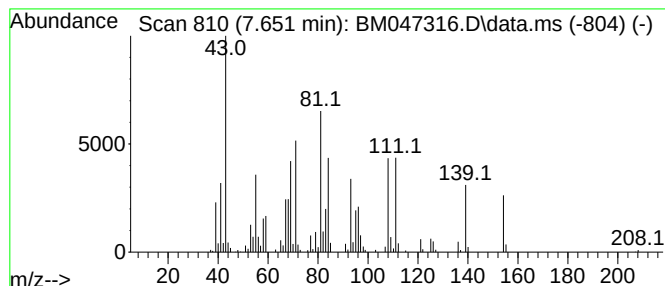
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.651	3.18 ng	228798	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	59
3			3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	38
4			Terpinen-4-ol	154	C10H18O	000562-74-3	35
5			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	22



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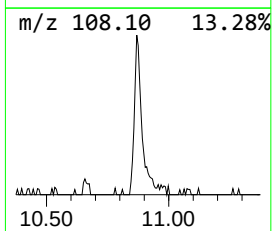
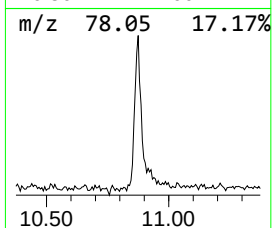
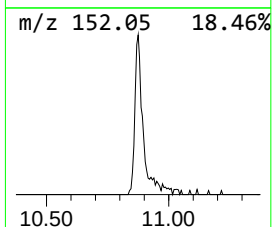
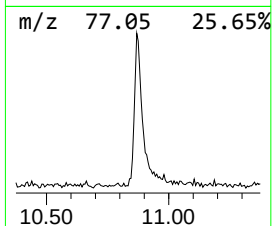
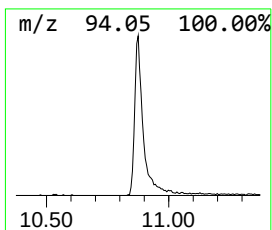
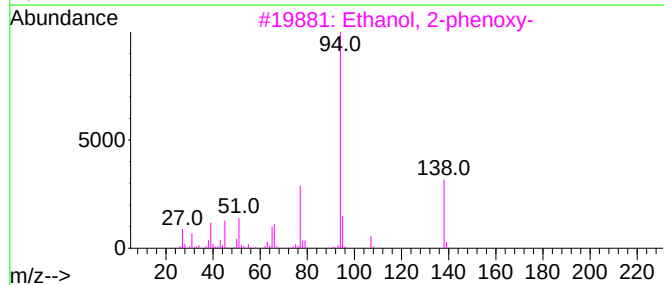
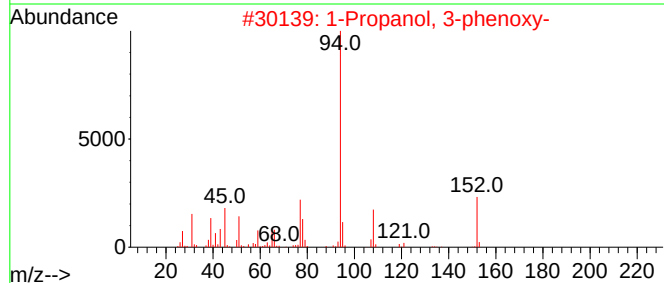
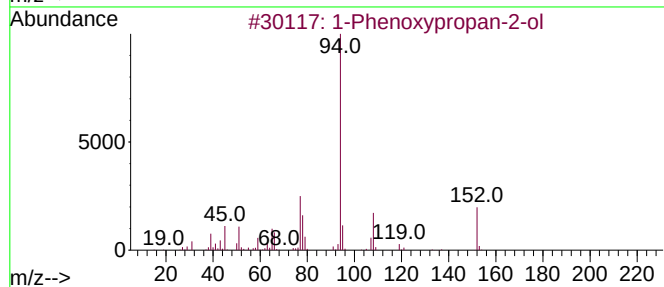
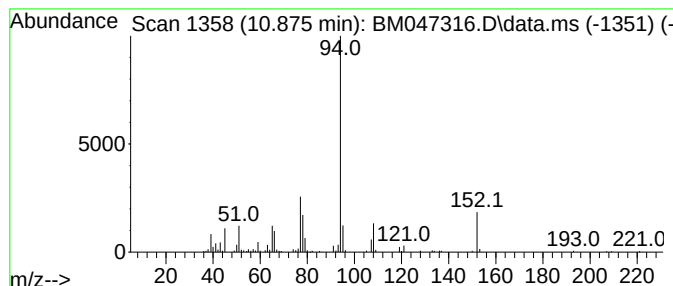
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.61 ng	258898	Naphthalene-d8	10.104

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	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			1,2-Propanediol, 3-phenoxy-	168	C9H12O3	000538-43-2	59



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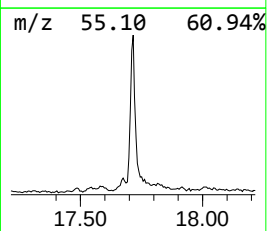
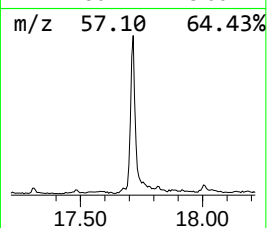
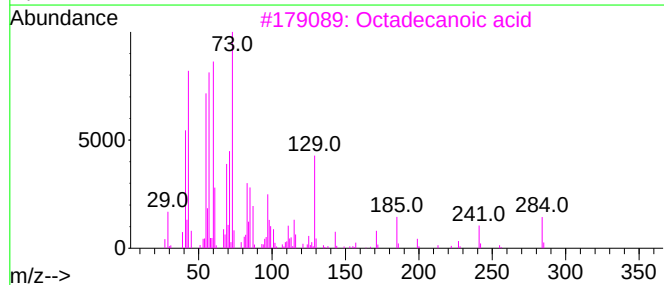
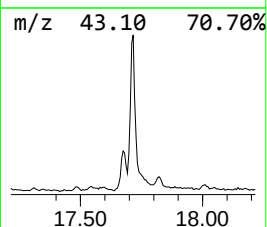
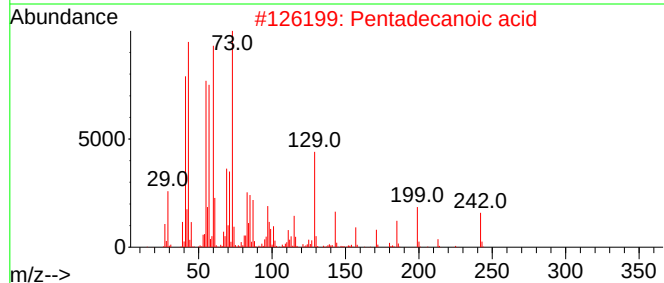
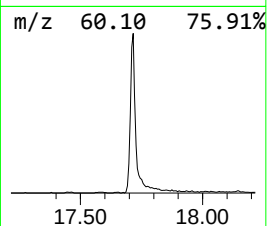
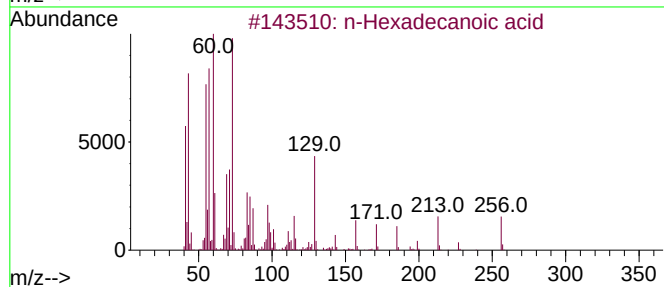
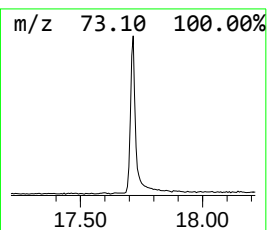
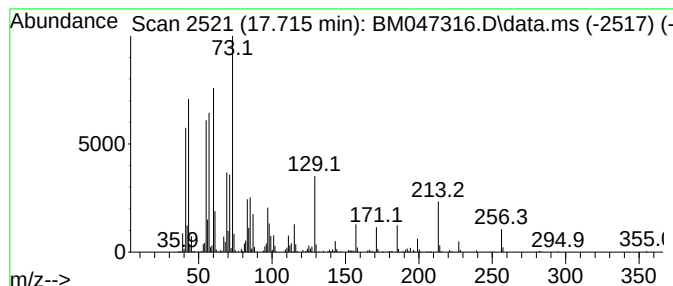
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	7.20 ng	1158600	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Octadecanoic acid	284	C18H36O2	000057-11-4	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047316.D
Acq On : 22 Aug 2024 14:31
Operator : RC/JU
Sample : P3671-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-912-J-SO-0-0.5-081924

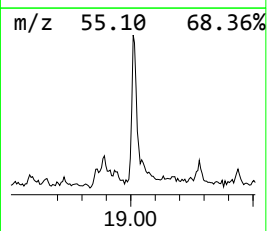
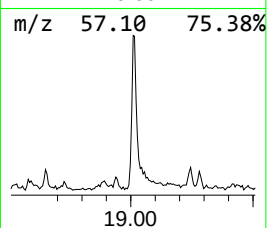
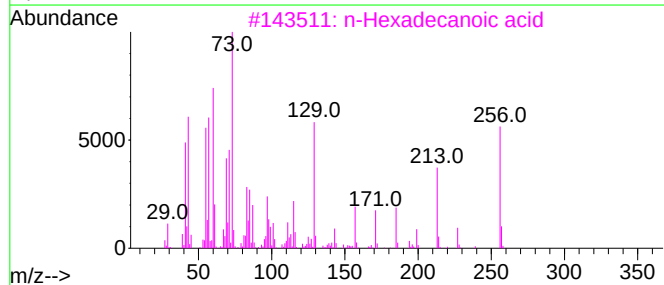
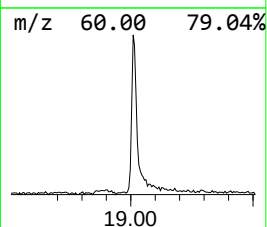
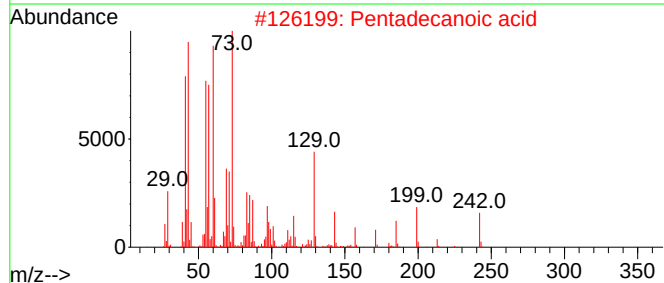
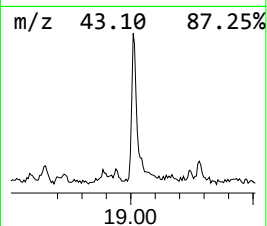
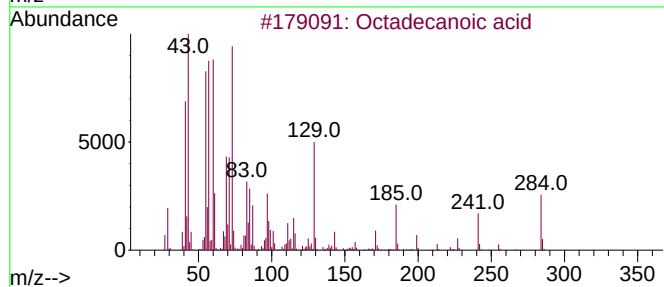
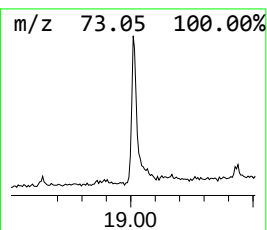
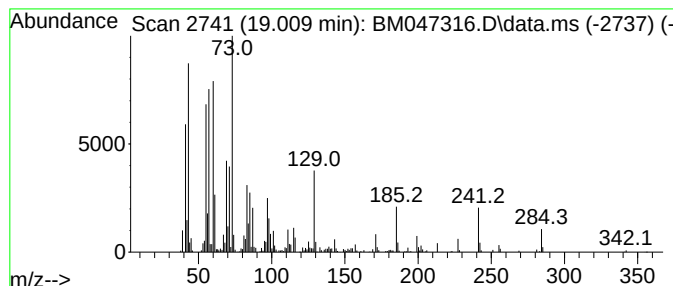
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	2.65 ng	473620	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047316.D
Acq On : 22 Aug 2024 14:31
Operator : RC/JU
Sample : P3671-13
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Instrument :
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ClientSampleId :
S-912-J-SO-0-0.5-081924

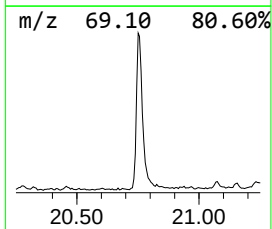
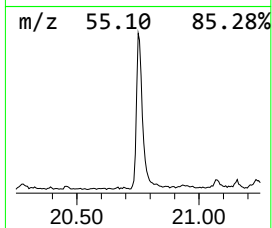
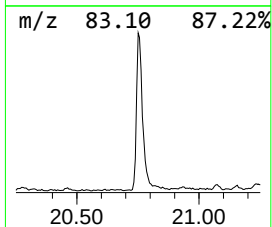
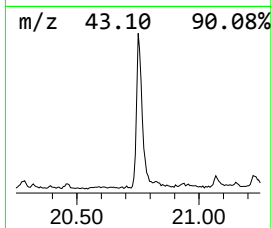
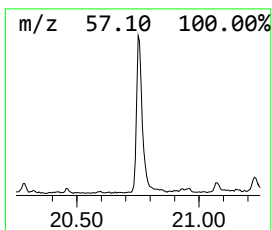
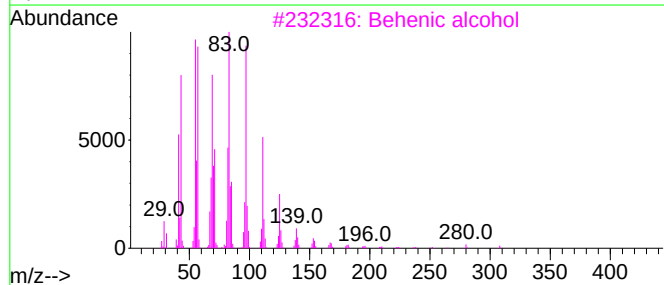
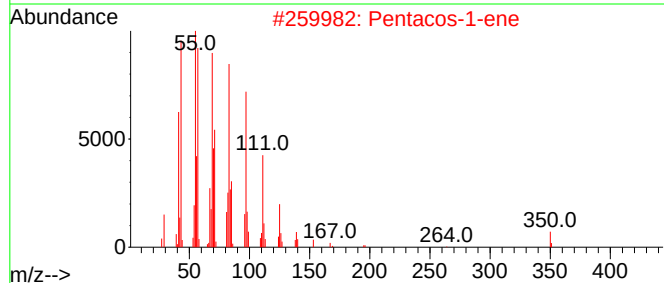
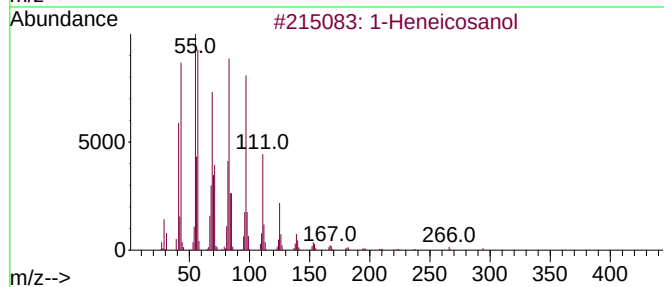
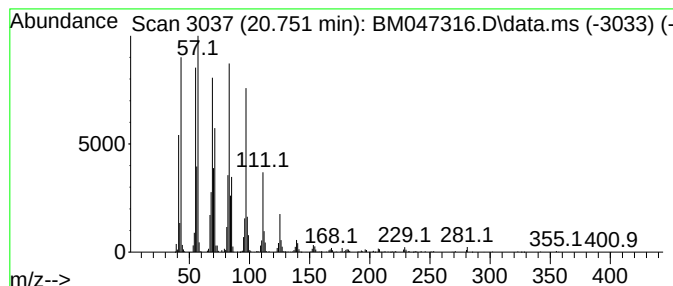
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.751	6.88 ng	1231840	Chrysene-d12	21.015

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Pentacos-1-ene	350	C25H50	016980-85-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047316.D
Acq On : 22 Aug 2024 14:31
Operator : RC/JU
Sample : P3671-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

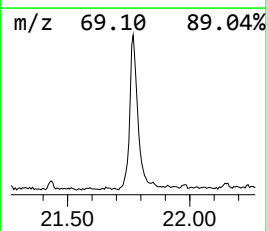
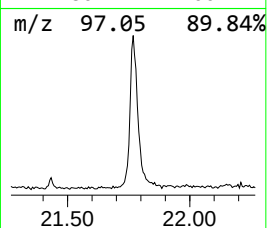
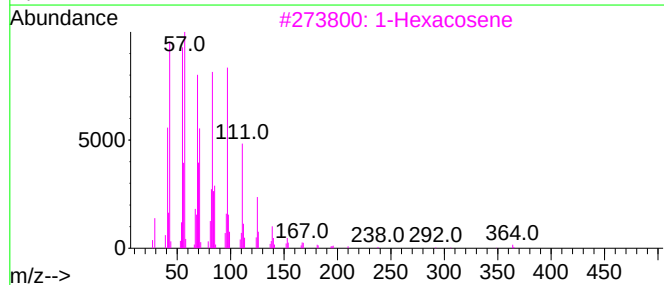
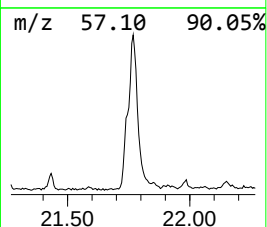
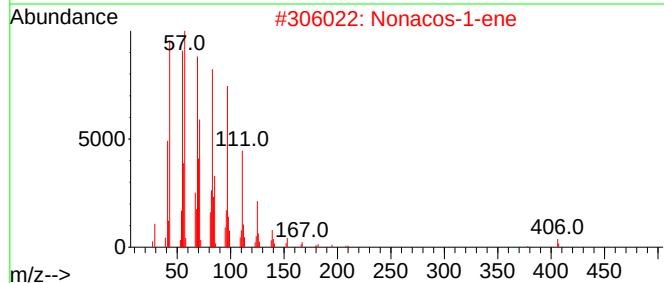
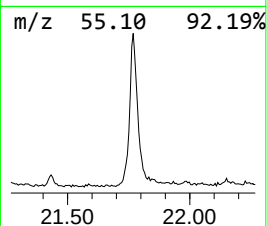
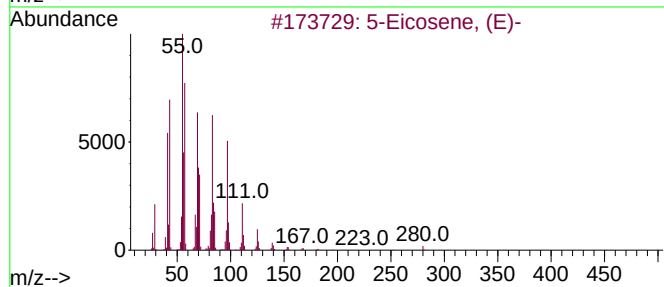
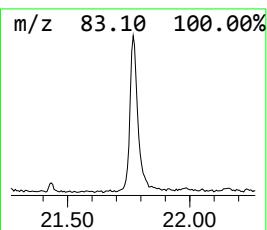
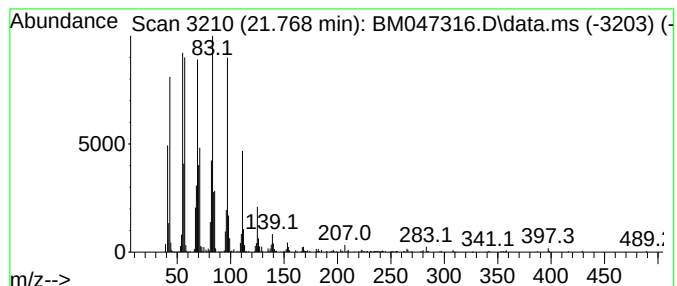
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ClientSampleId :
S-912-J-SO-0-0.5-081924

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 8 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.768	6.97 ng	1247360	Chrysene-d12		21.015	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	Nonacos-1-ene		406	C29H58	018835-35-3	95
3	1-Hexacosene		364	C26H52	018835-33-1	95
4	Behenic alcohol		326	C22H46O	000661-19-8	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047316.D
Acq On : 22 Aug 2024 14:31
Operator : RC/JU
Sample : P3671-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-912-J-SO-0-0.5-081924

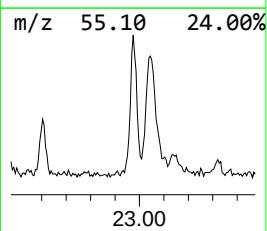
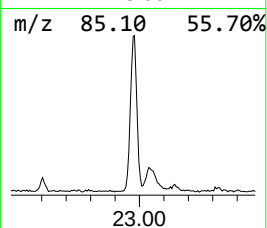
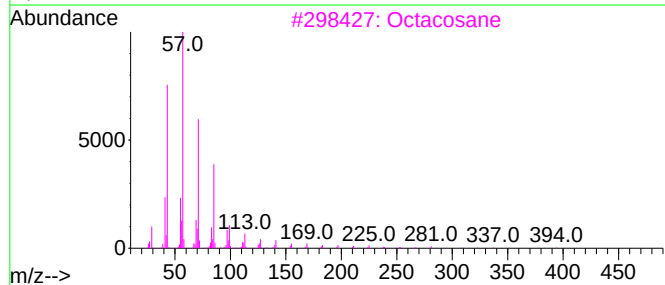
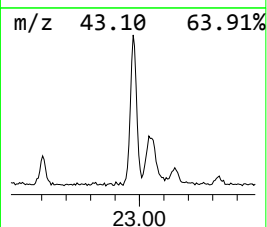
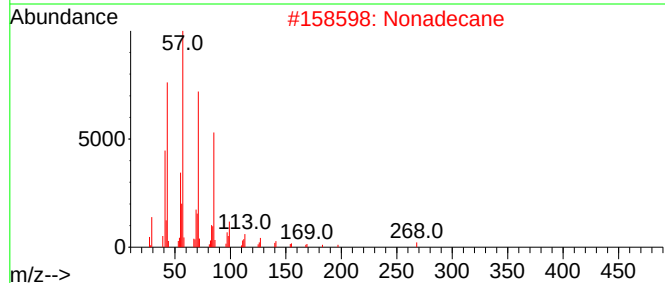
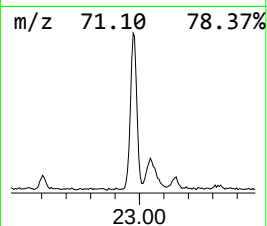
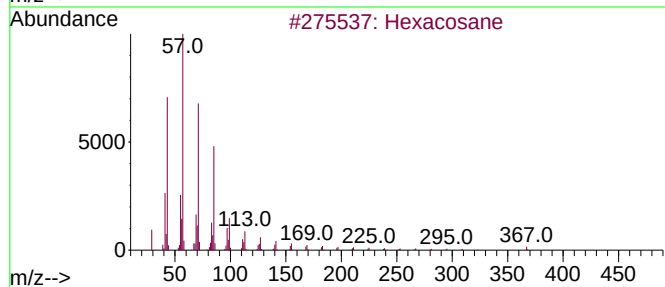
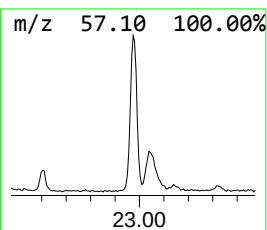
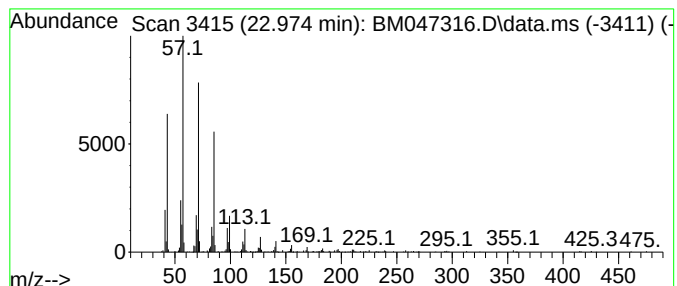
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.974	2.92 ng	504368	Perylene-d12	23.709

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	94
2		Nonadecane	268	C19H40	000629-92-5	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047316.D
Acq On : 22 Aug 2024 14:31
Operator : RC/JU
Sample : P3671-13
Misc :
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S-912-J-SO-0-0.5-081924

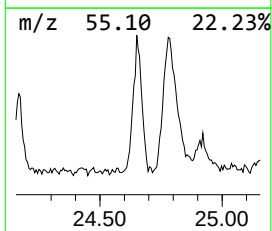
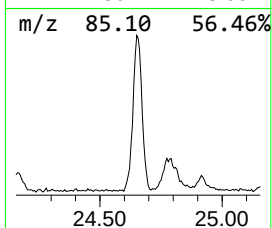
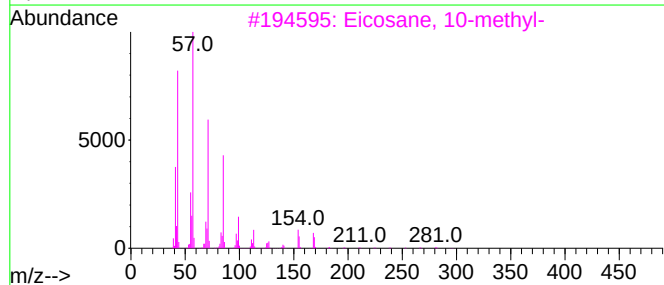
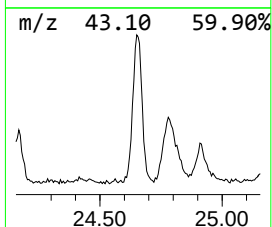
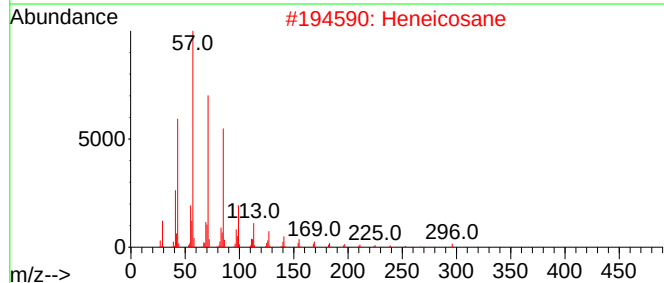
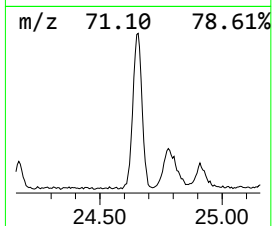
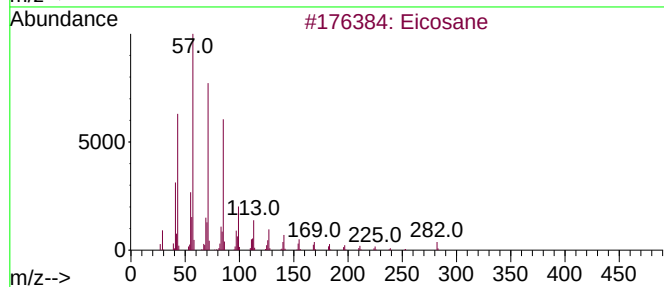
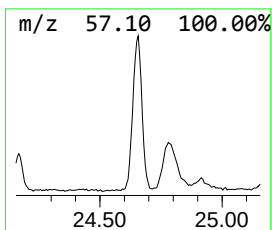
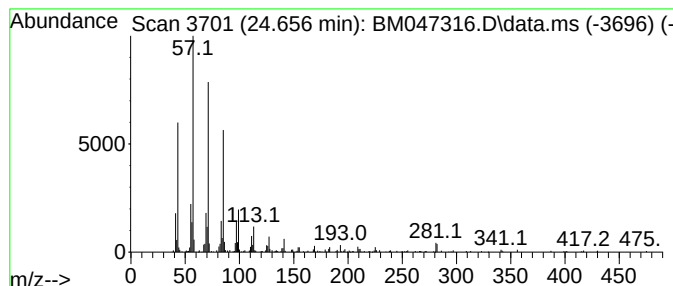
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.656	3.87 ng	668227	Perylene-d12	23.709

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047316.D
Acq On : 22 Aug 2024 14:31
Operator : RC/JU
Sample : P3671-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-912-J-SO-0-0.5-081924

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	4.563	3.8	ng	273972	1	7.351	1440390	20.0
Eucalyptol	7.651	3.2	ng	228798	1	7.351	1440390	20.0
1-Phenoxypropan...	10.875	2.6	ng	258898	2	10.104	1987500	20.0
n-Hexadecanoic ...	17.715	7.2	ng	1158600	4	16.774	3216700	20.0
Octadecanoic acid	19.009	2.6	ng	473620	5	21.015	3578340	20.0
1-Heneicosanol	20.751	6.9	ng	1231840	5	21.015	3578340	20.0
5-Eicosene, (E)-	21.768	7.0	ng	1247360	5	21.015	3578340	20.0
Hexacosane	22.974	2.9	ng	504368	6	23.709	3455110	20.0
Eicosane	24.656	3.9	ng	668227	6	23.709	3455110	20.0