

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061322\
 Data File : BM035462.D
 Acq On : 13 Jun 2022 18:02
 Operator : CG/JU
 Sample : N3324-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BT-SPOILS-07

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-BM061022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.557	77	80	95	rVB	91984	176193	1.43%	0.262%
2	4.940	308	315	325	rBV	203795	322244	2.61%	0.480%
3	5.404	388	394	415	rBV	4717517	7093900	57.41%	10.562%
4	6.169	519	524	536	rBV	105139	185582	1.50%	0.276%
5	7.004	656	666	692	rBV	4402078	7455687	60.34%	11.101%
6	7.816	798	804	817	rBV	725031	1211255	9.80%	1.803%
7	8.981	991	1002	1013	rBV	2722684	4660498	37.72%	6.939%
8	10.616	1270	1280	1297	rBV	959064	1770672	14.33%	2.636%
9	13.086	1693	1700	1721	rBV	6342378	9573740	77.48%	14.254%
10	14.463	1927	1934	1947	rVB	1351960	2094372	16.95%	3.118%
11	15.951	2179	2187	2211	rBV	4647271	7157003	57.92%	10.656%
12	17.204	2395	2400	2414	rBV	1530588	2328554	18.84%	3.467%
13	18.115	2550	2555	2568	rBV	795687	1295422	10.48%	1.929%
14	19.392	2768	2772	2789	rBV	426356	709829	5.74%	1.057%
15	19.833	2841	2847	2856	rBV	9928664	12356869	100.00%	18.398%
16	21.109	3059	3064	3074	rBV	1663636	2341561	18.95%	3.486%
17	21.392	3107	3112	3124	rBV	2198300	3017605	24.42%	4.493%
18	21.550	3136	3139	3146	rBV2	116117	160605	1.30%	0.239%
19	23.733	3504	3510	3523	rVB	1662949	3253397	26.33%	4.844%

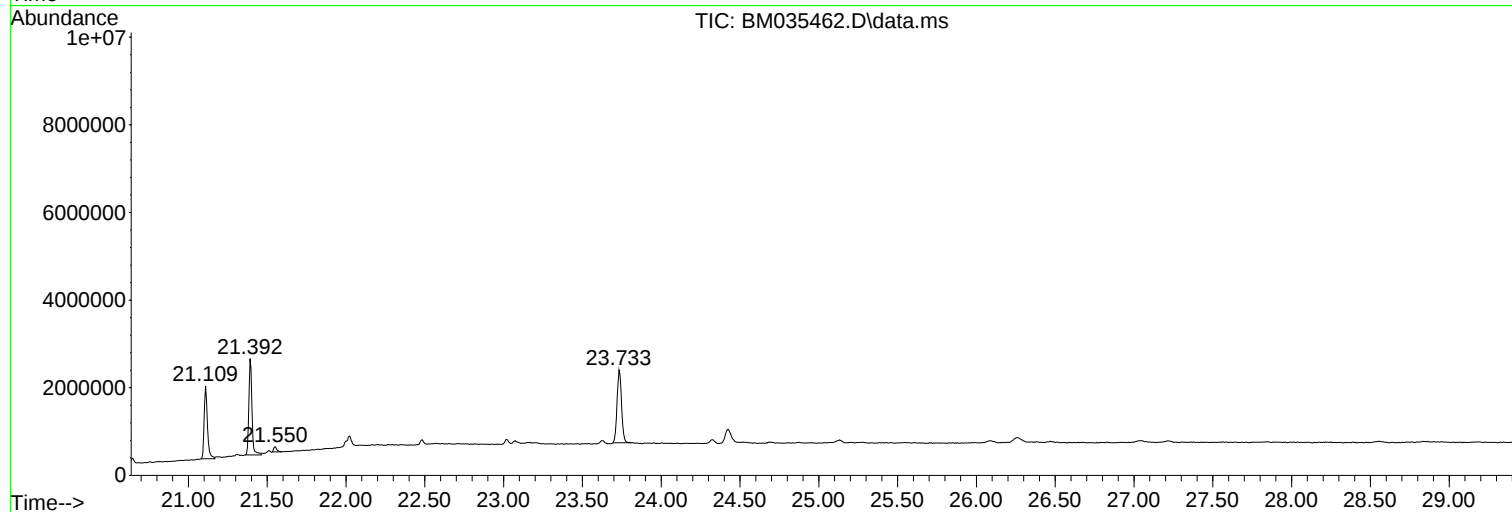
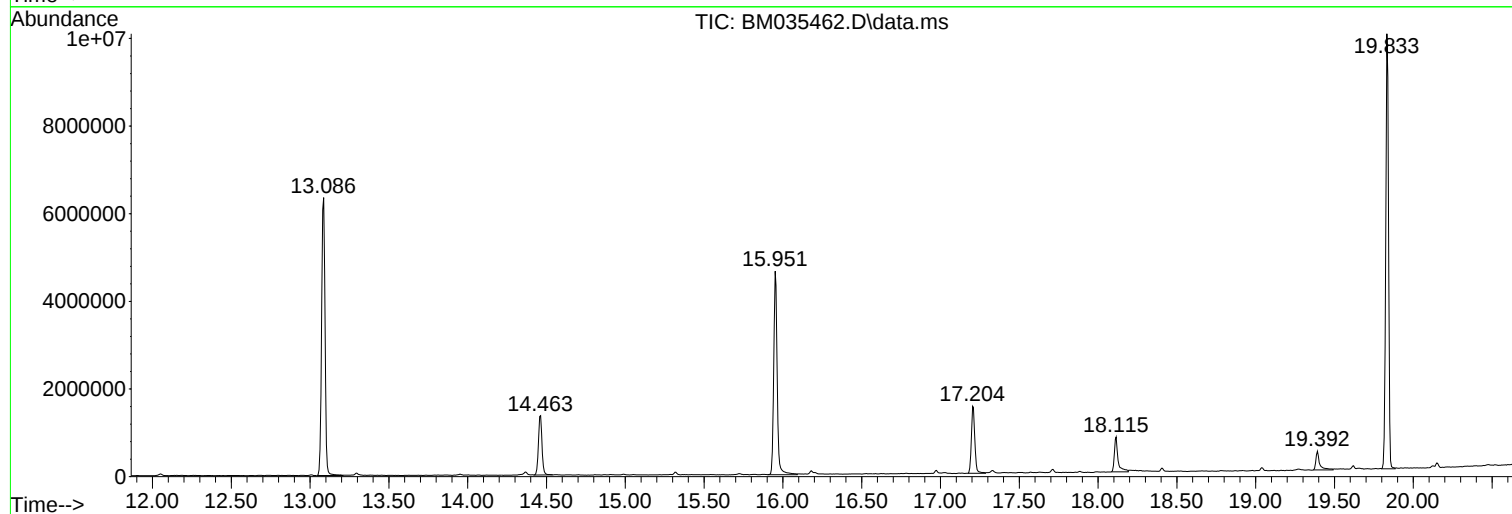
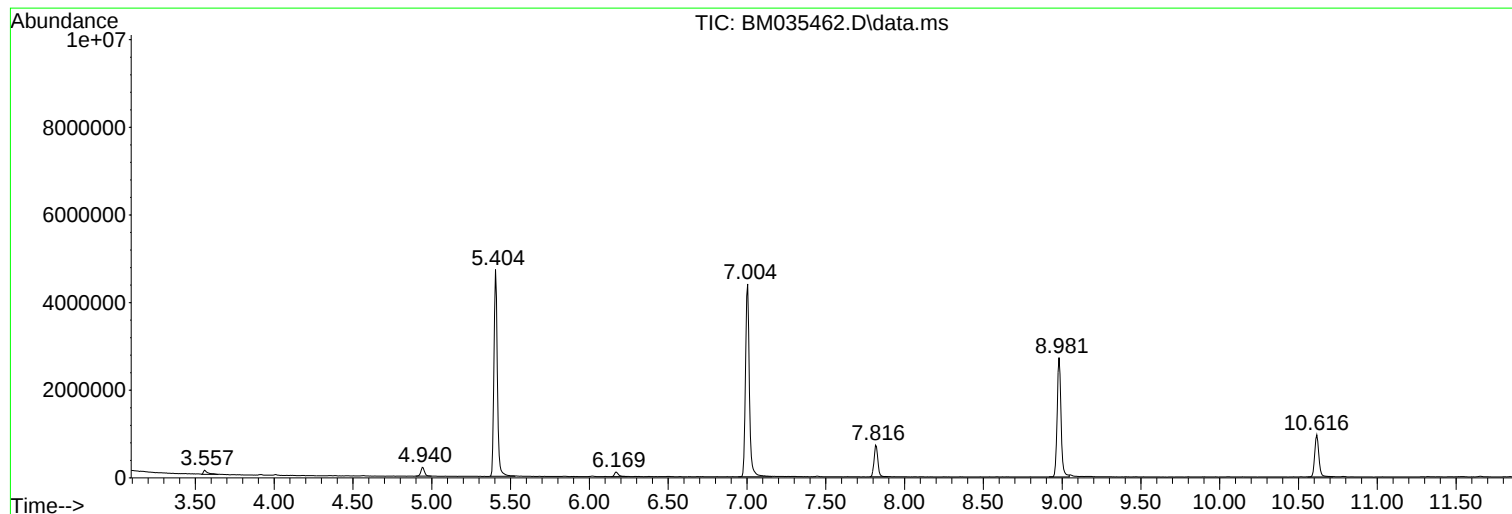
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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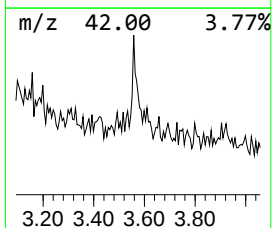
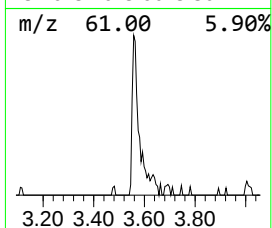
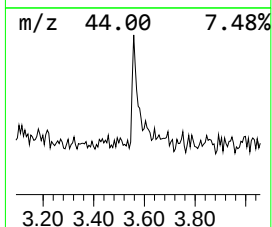
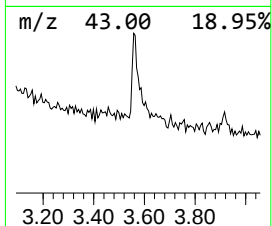
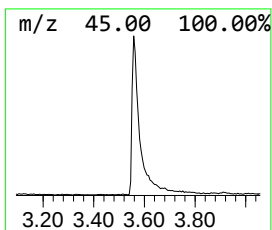
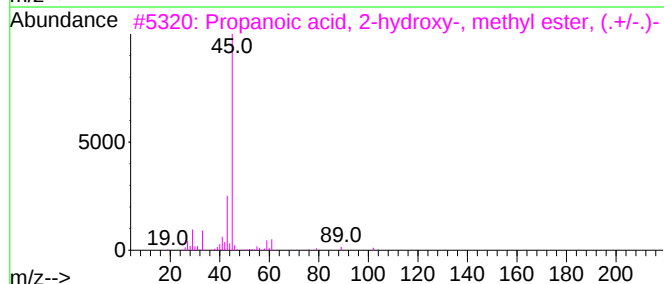
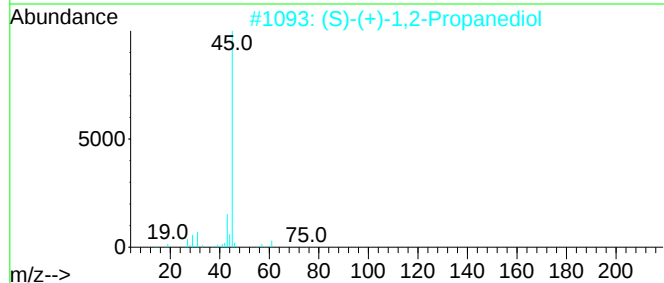
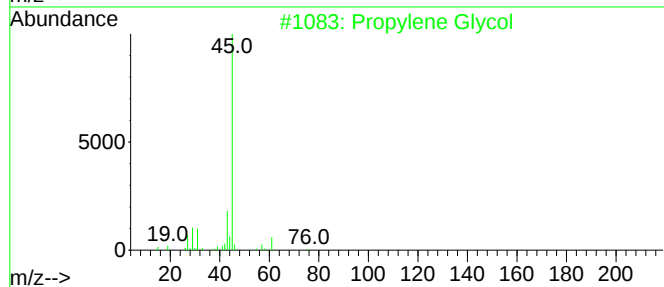
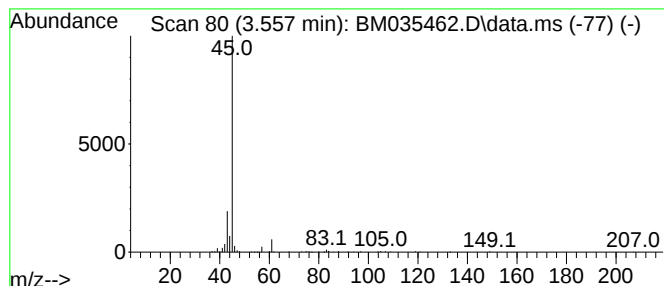
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.557	2.91 ng	176193	1,4-Dichlorobenzene-d4	7.816

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	56
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	56
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5			3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	40



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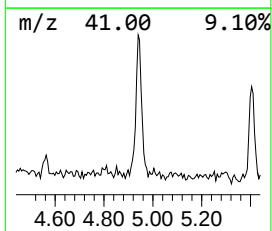
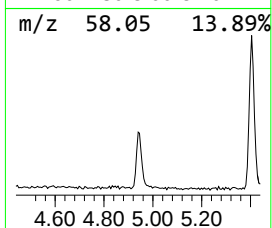
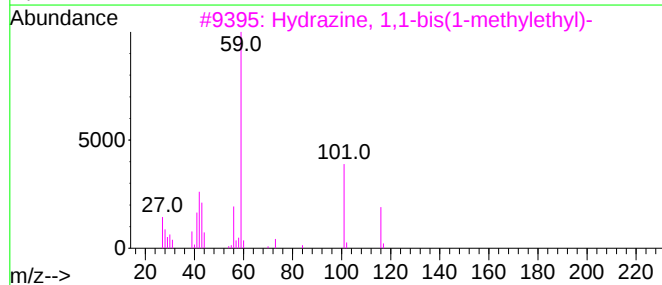
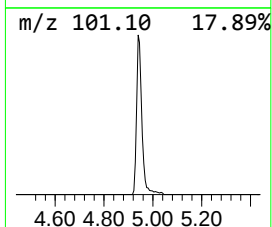
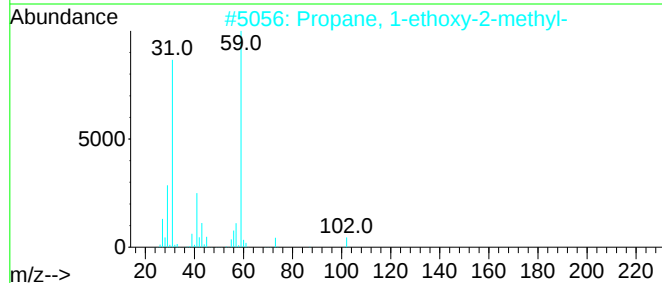
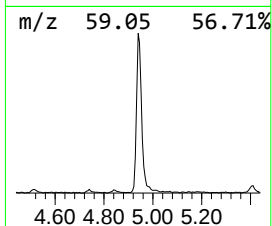
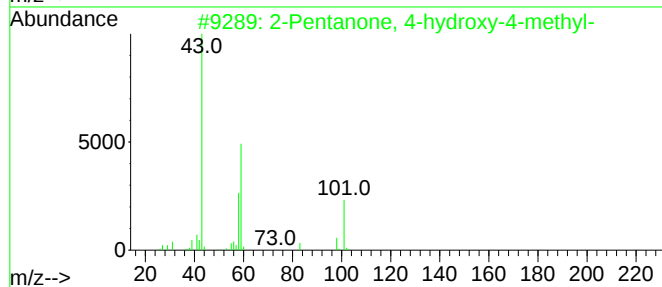
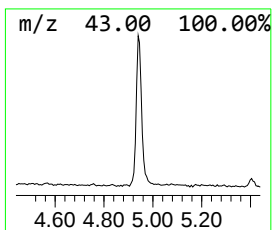
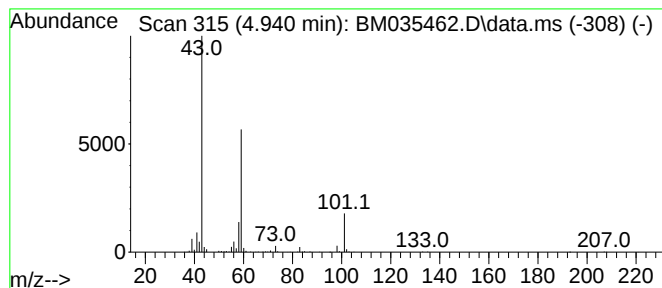
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.940	5.32 ng	322244	1,4-Dichlorobenzene-d4			7.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O		000627-02-1	37
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2		000921-14-2	28
4	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	25
5	Hexaethylene glycol dimethyl ether	310	C14H30O7		001072-40-8	25



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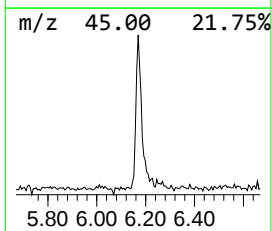
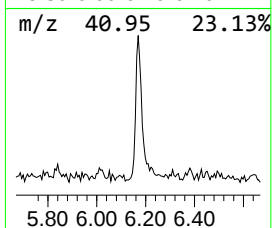
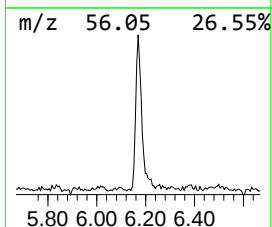
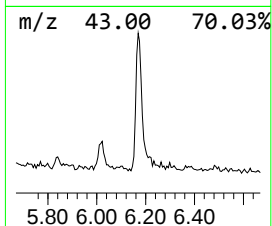
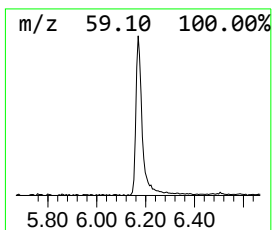
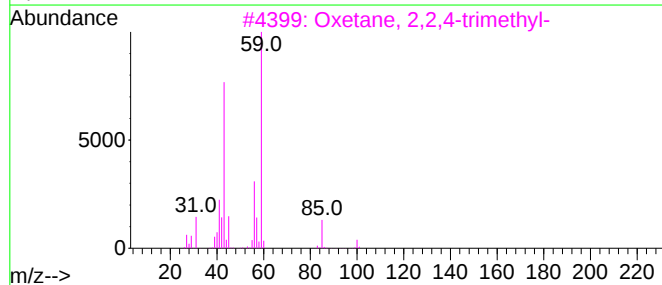
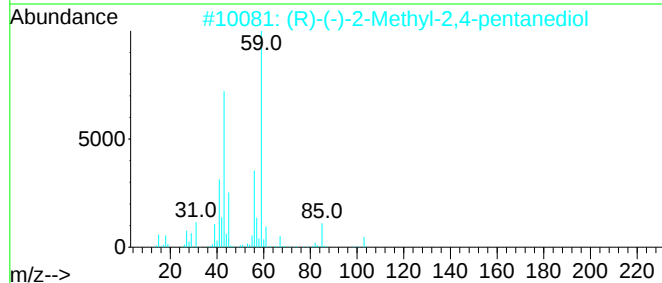
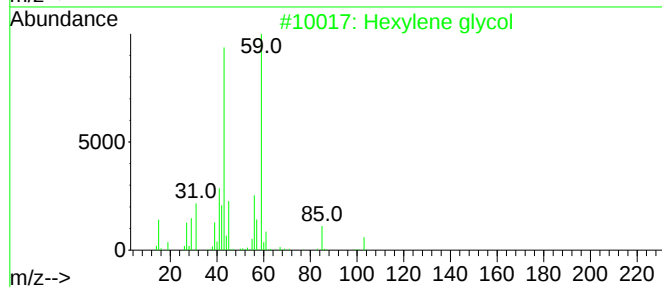
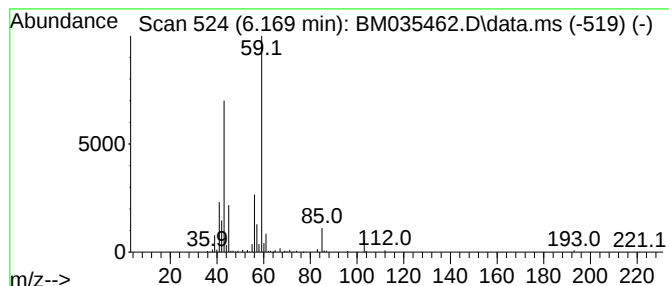
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.169	3.06 ng	185582	1,4-Dichlorobenzene-d4	7.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexylene glycol	118	C6H14O2	000107-41-5	90
2			(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	78
3			Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	72
4			2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	58
5			2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	47



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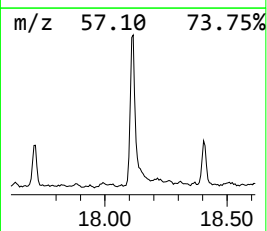
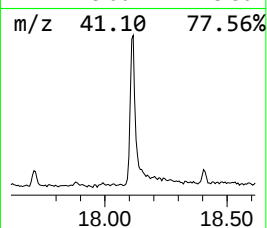
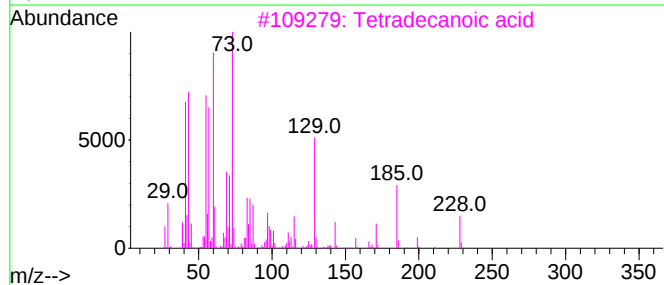
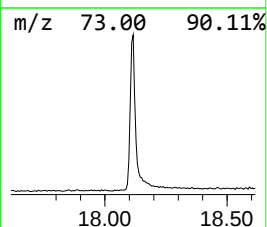
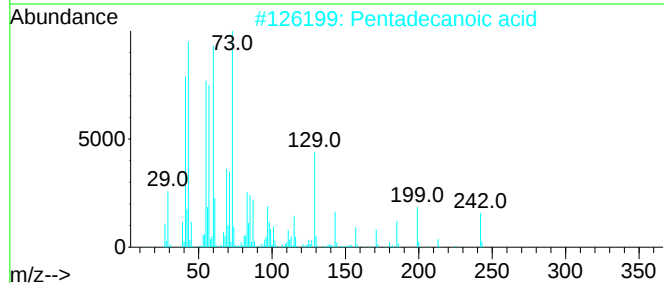
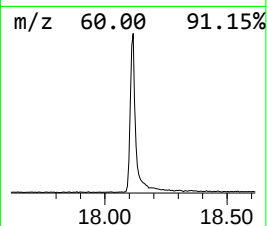
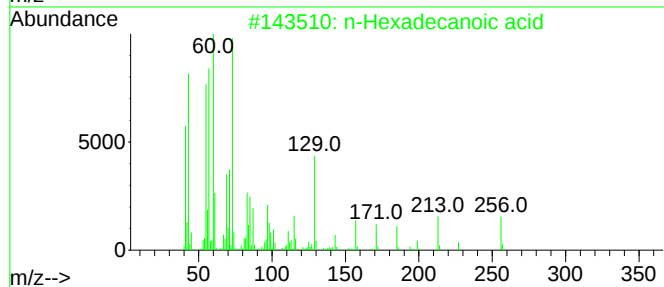
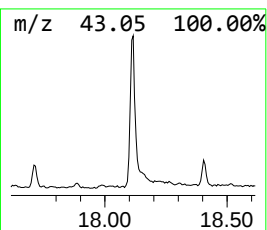
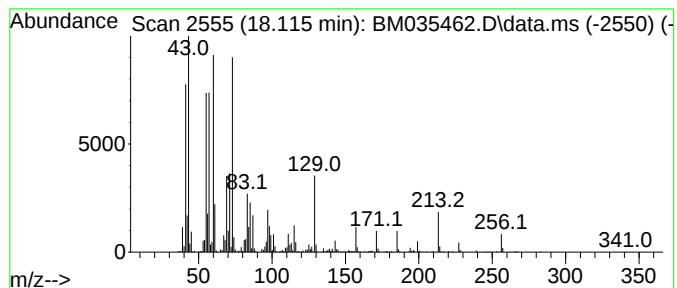
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	11.13 ng	1295420	Phenanthrene-d10	17.204

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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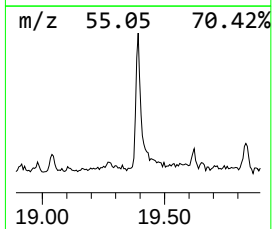
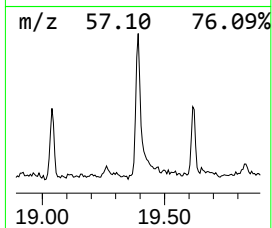
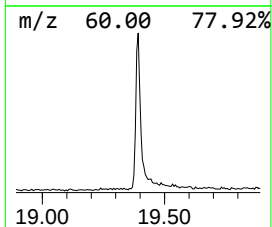
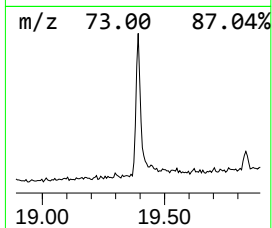
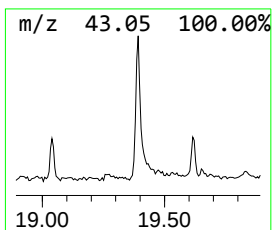
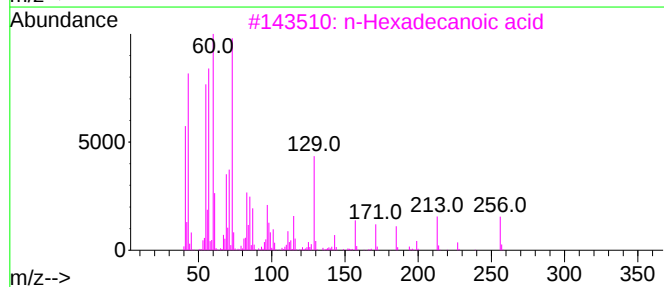
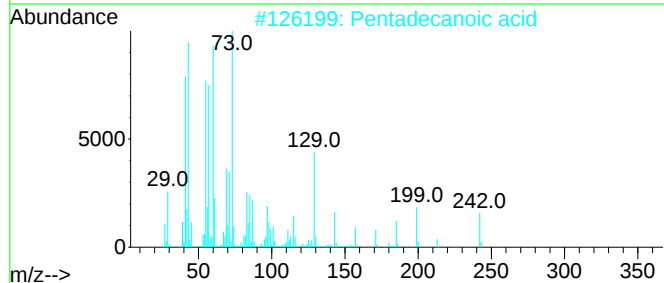
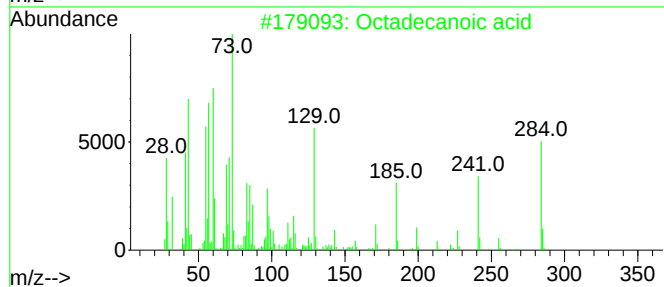
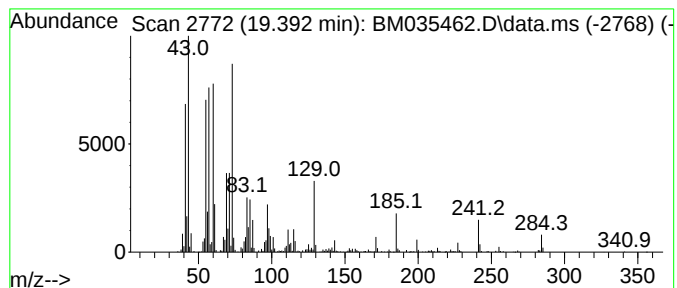
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.392	4.70 ng	709829	Chrysene-d12	21.392

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	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



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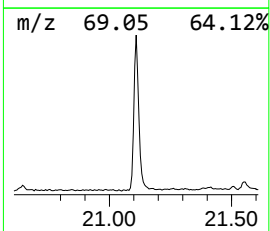
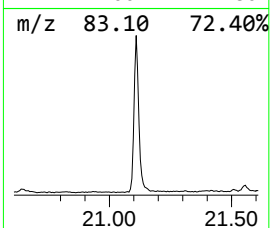
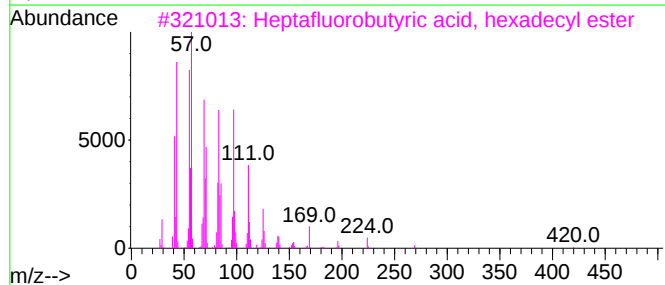
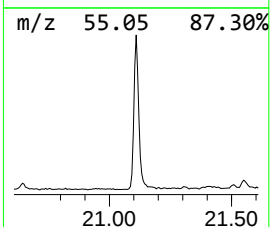
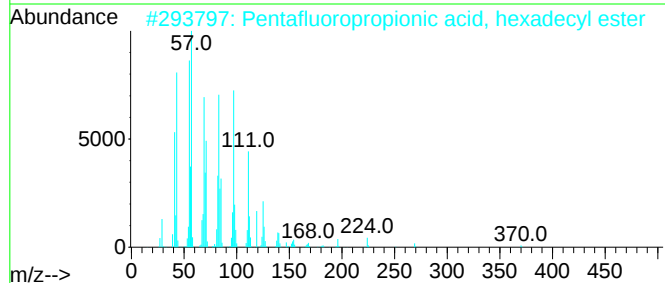
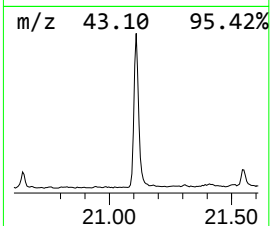
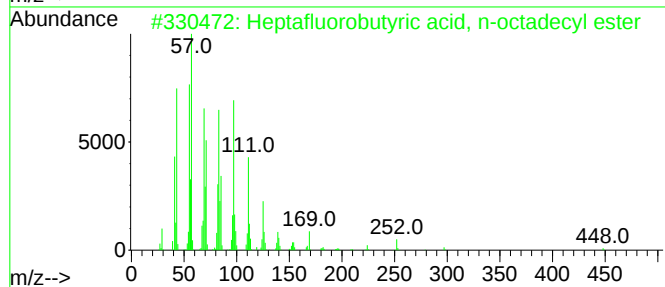
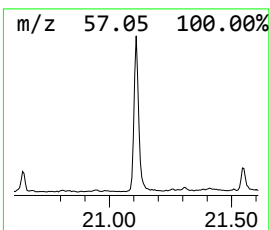
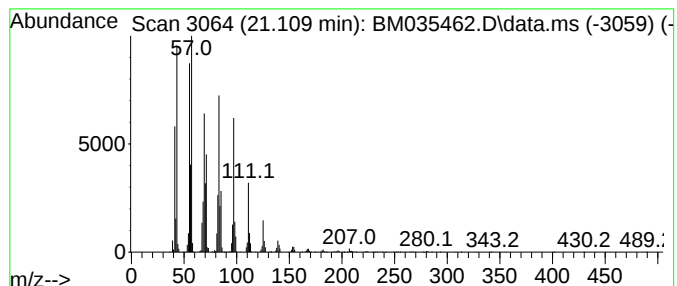
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.109	15.52 ng	2341560	Chrysene-d12	21.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
2			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061322\
Data File : BM035462.D
Acq On : 13 Jun 2022 18:02
Operator : CG/JU
Sample : N3324-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BT-SPOILS-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061022.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
Propylene Glycol	3.557	2.9	ng	176193	1	7.816	1211260	20.0
2-Pentanone, 4-...	4.940	5.3	ng	322244	1	7.816	1211260	20.0
Hexylene glycol	6.169	3.1	ng	185582	1	7.816	1211260	20.0
n-Hexadecanoic ...	18.115	11.1	ng	1295420	4	17.204	2328550	20.0
Octadecanoic acid	19.392	4.7	ng	709829	5	21.392	3017610	20.0
Heptafluorobuty...	21.109	15.5	ng	2341560	5	21.392	3017610	20.0