

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
 Data File : BG054329.D
 Acq On : 20 Jul 2022 15:58
 Operator : CG/JU
 Sample : N3771-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-7F

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_G\Methods\8270-BG071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.565	363	370	381	rVB	135026	235507	10.83%	2.905%
2	7.163	635	642	652	rBV	90600	157080	7.22%	1.938%
3	7.991	777	783	790	rBV	57617	98574	4.53%	1.216%
4	9.154	974	981	993	rVB	201711	382735	17.60%	4.722%
5	10.565	1215	1221	1233	rBB3	13913	24650	1.13%	0.304%
6	10.800	1253	1261	1271	rBB	77944	139582	6.42%	1.722%
7	13.250	1671	1678	1687	rBV	662731	1061618	48.82%	13.097%
8	14.625	1905	1912	1919	rBV	139746	230581	10.60%	2.845%
9	16.117	2159	2166	2179	rBV2	704282	1103340	50.74%	13.612%
10	17.374	2372	2380	2388	rBV	214637	324433	14.92%	4.003%
11	18.267	2527	2532	2542	rBV2	24854	44932	2.07%	0.554%
12	19.536	2743	2748	2755	rBV2	20657	34810	1.60%	0.429%
13	19.983	2818	2824	2830	rBV	1604540	2174341	100.00%	26.825%
14	21.405	3060	3066	3071	rBV6	21847	48062	2.21%	0.593%
15	21.640	3099	3106	3113	rVB	260951	429751	19.76%	5.302%
16	23.097	3346	3354	3361	rVB2	56605	116082	5.34%	1.432%
17	23.303	3384	3389	3398	rVB2	13155	27674	1.27%	0.341%
18	24.836	3639	3650	3662	rVB2	309202	852928	39.23%	10.523%
19	27.298	4056	4069	4085	rVB4	93891	392139	18.03%	4.838%
20	30.870	4662	4677	4693	rVB6	41018	226803	10.43%	2.798%

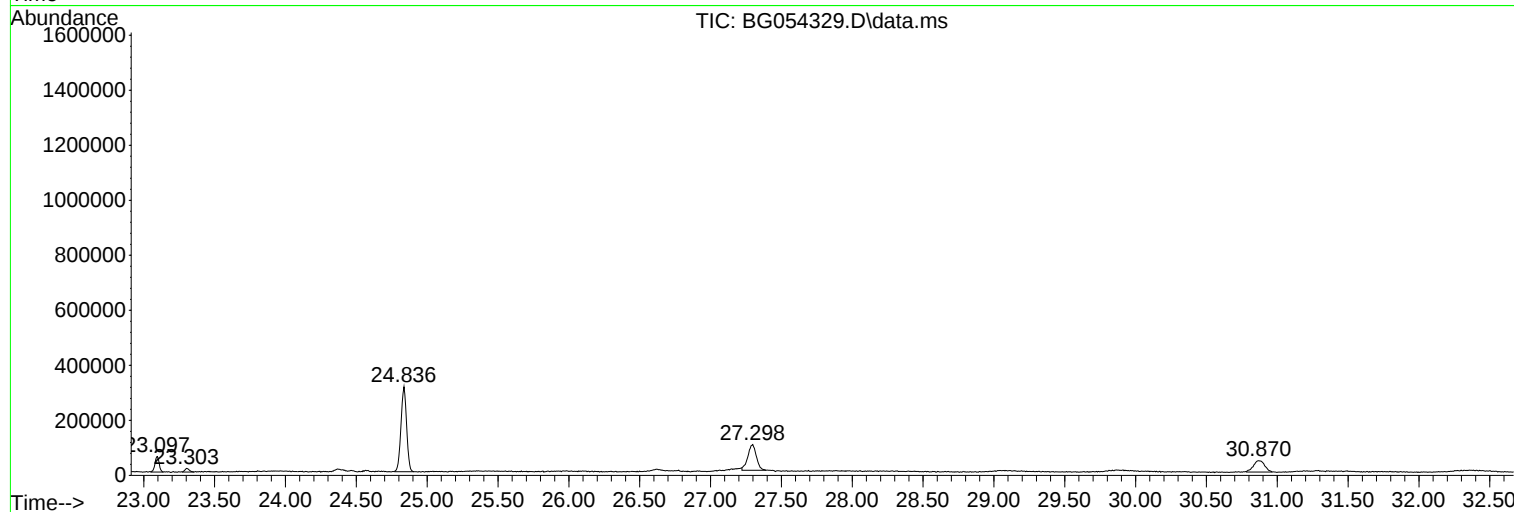
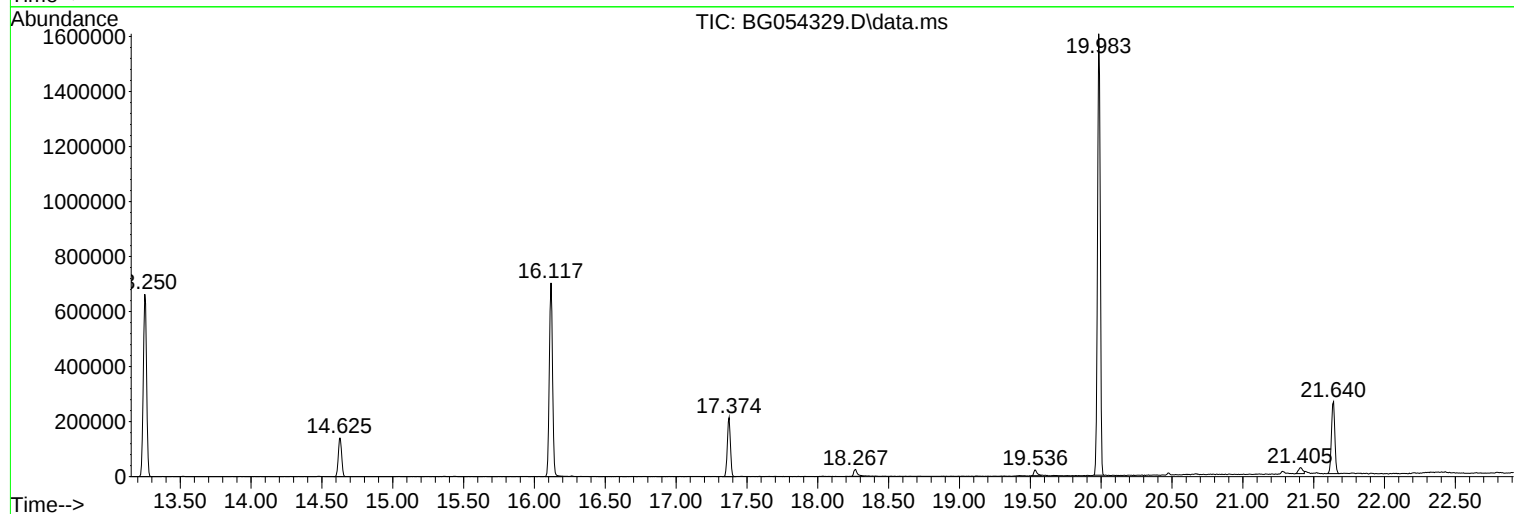
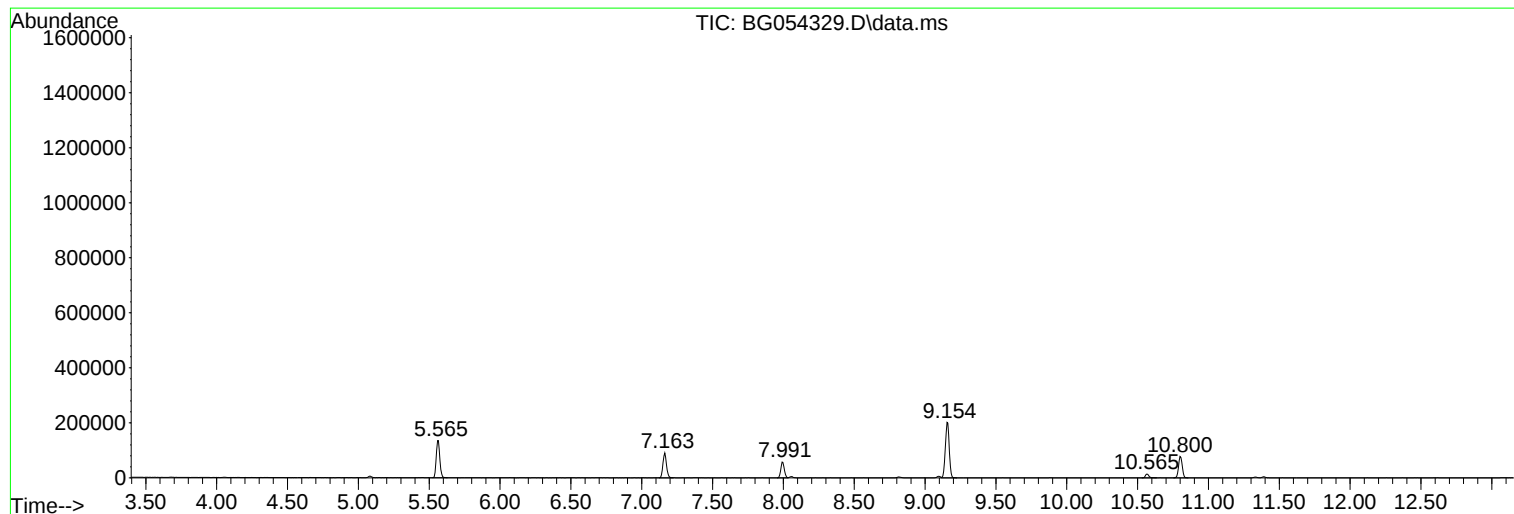
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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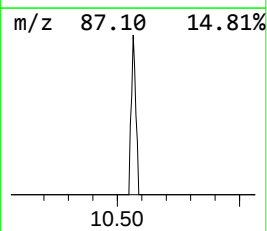
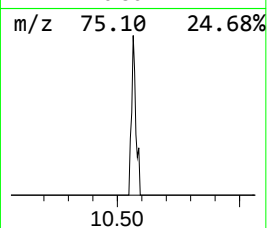
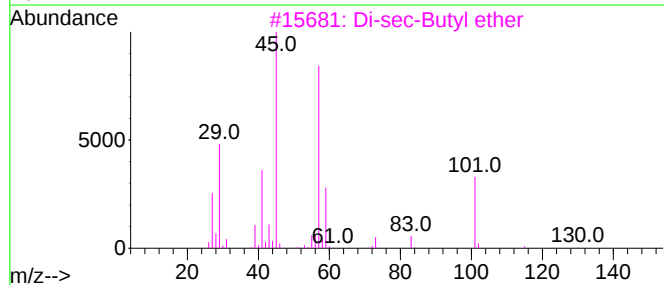
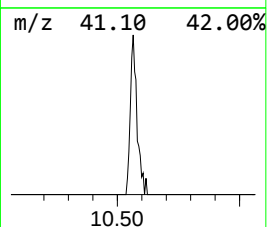
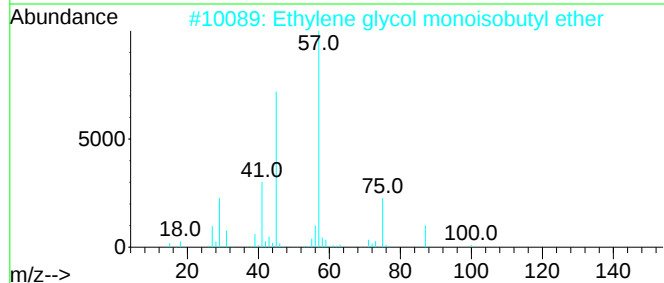
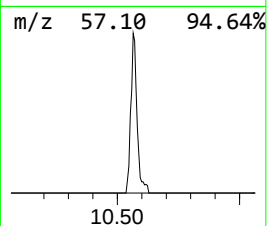
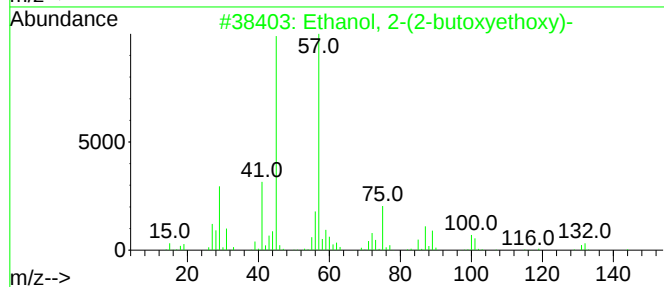
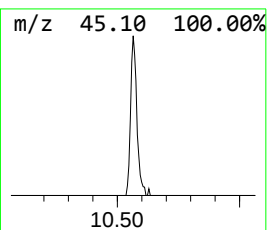
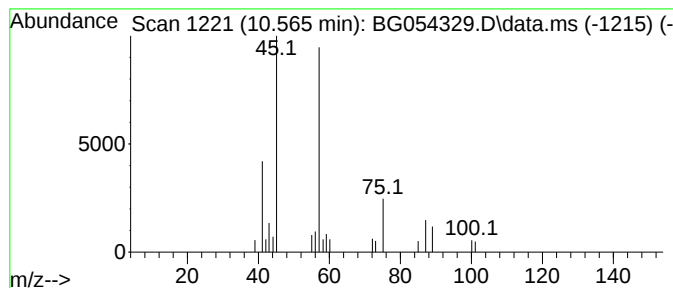
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.565	3.53 ng	24650	Naphthalene-d8	10.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	40
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	40
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	40



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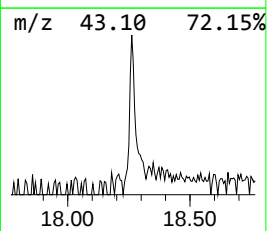
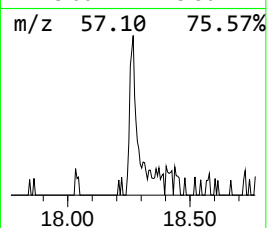
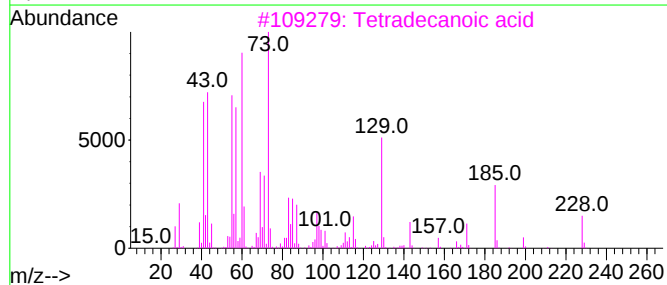
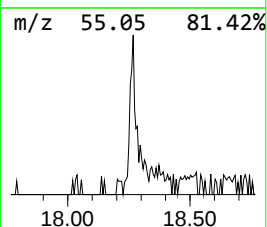
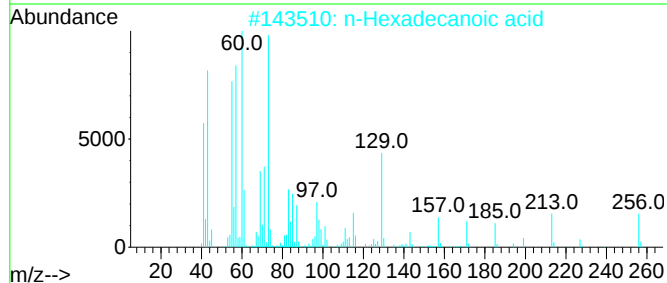
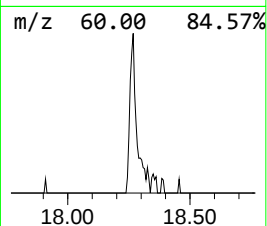
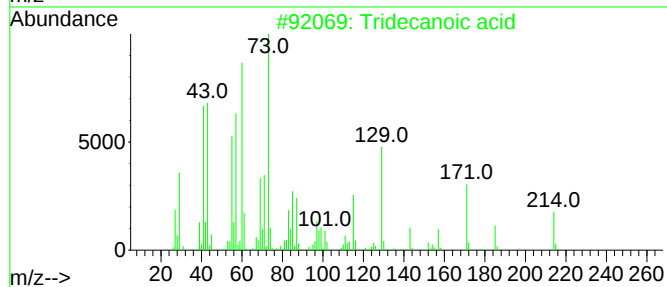
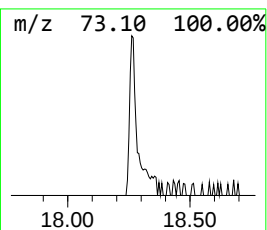
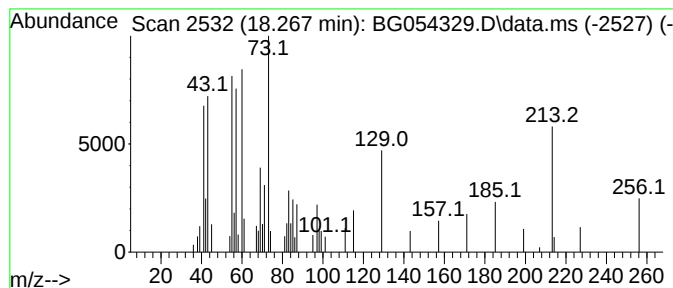
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.267	2.77 ng	44932	Phenanthrene-d10	17.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	47



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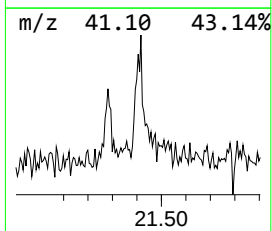
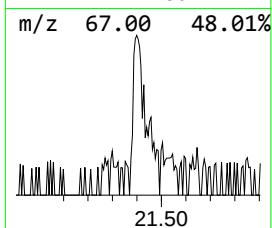
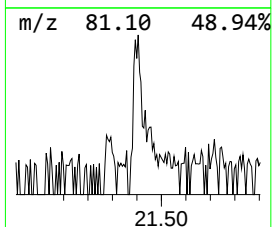
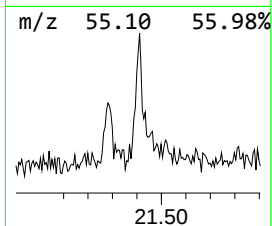
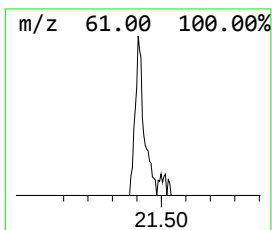
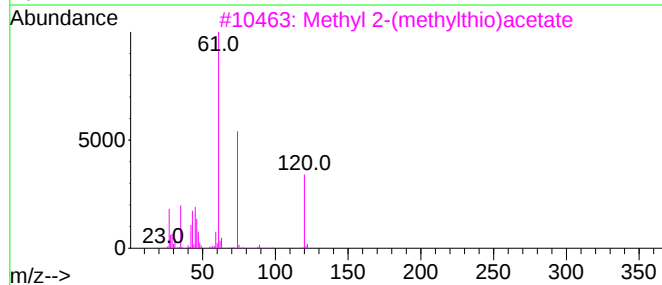
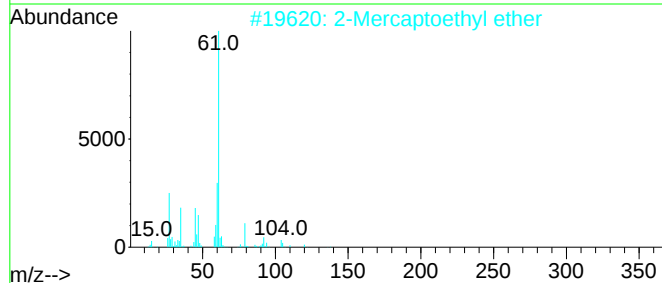
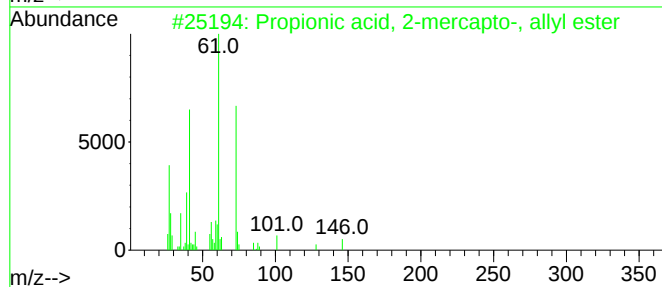
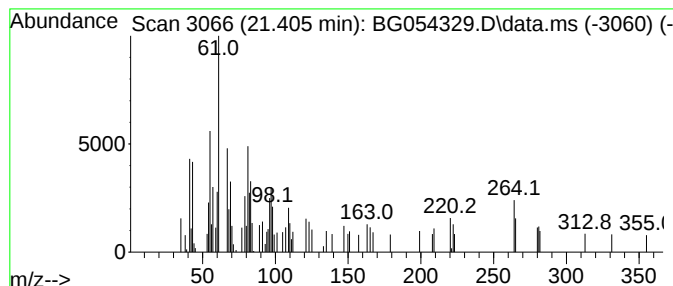
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Peak Number 3 unknown21.405 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.405	2.24 ng	48062	Chrysene-d12	21.640

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propionic acid, 2-mercapto-, all...	146	C6H10O2S	016883-50-4	25
2			2-Mercaptoethyl ether	138	C4H10O2S	002150-02-9	25
3			Methyl 2-(methylthio)acetate	120	C4H8O2S	016630-66-3	17
4			.alpha.-d-Xylopyranoside, 2,4-O...	202	C8H15B05	061553-47-7	16
5			9-Octadecenoic acid	282	C18H34O2	002027-47-6	15



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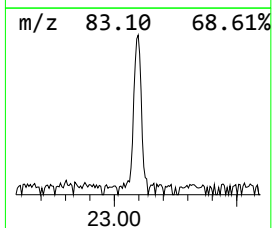
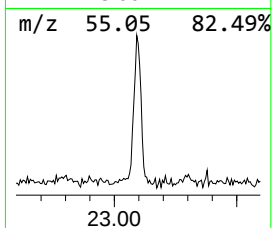
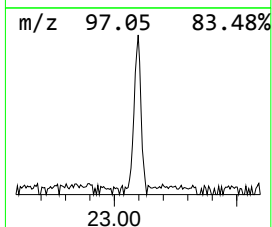
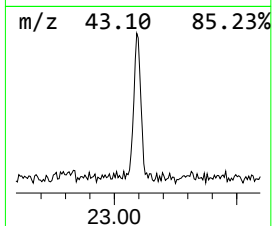
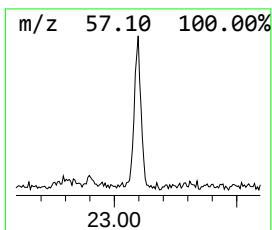
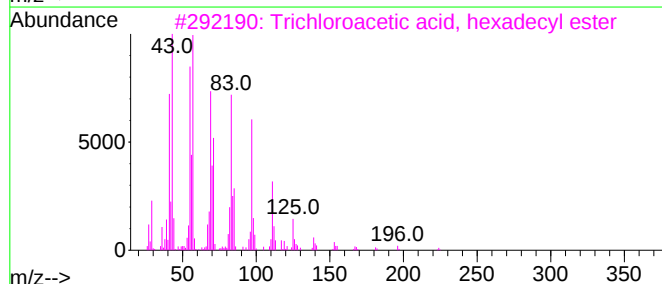
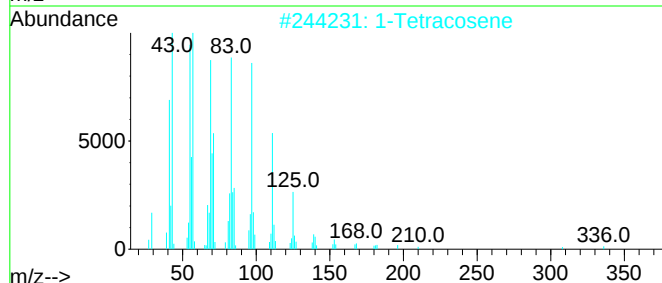
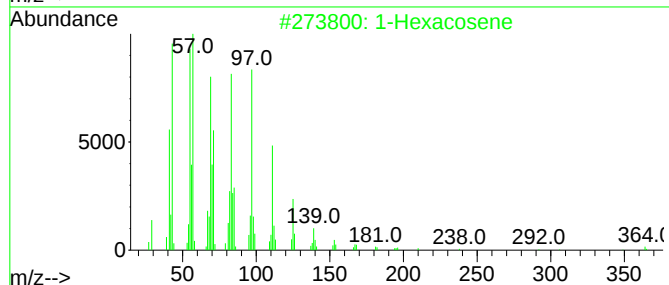
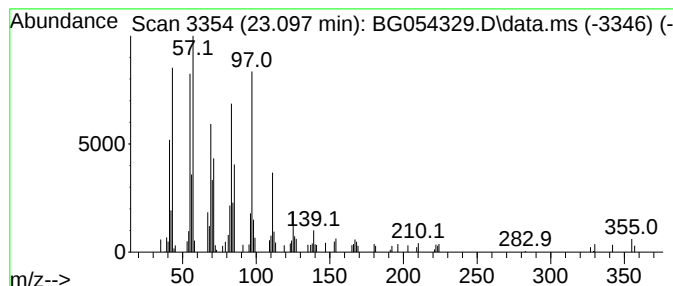
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Peak Number 4 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.097	5.40 ng	116082	Chrysene-d12	21.640

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	93
2	1-Tetracosene			336	C24H48	010192-32-2	93
3	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	92
4	Octacosanol			410	C28H58O	000557-61-9	91
5	1-Heneicosanol			312	C21H44O	015594-90-8	91



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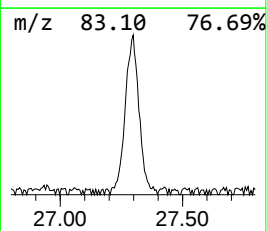
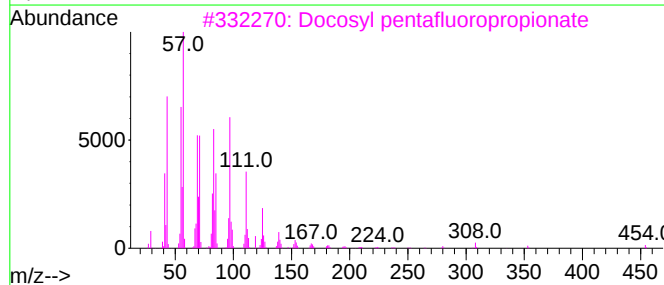
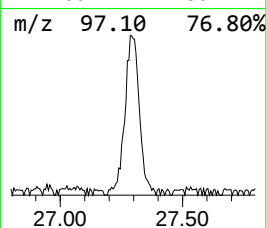
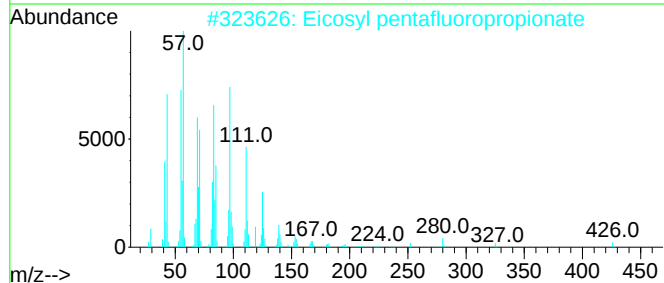
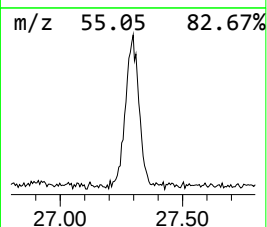
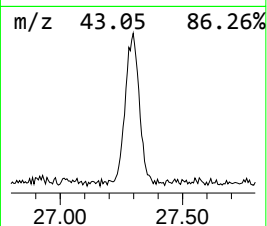
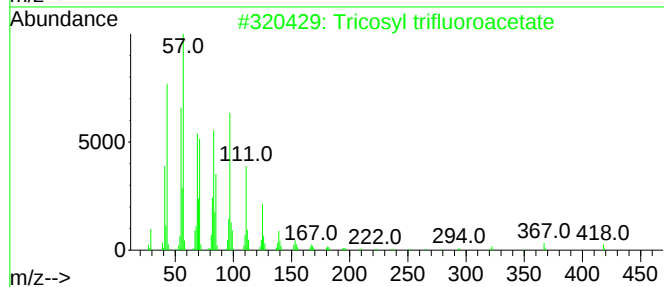
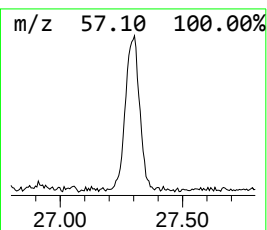
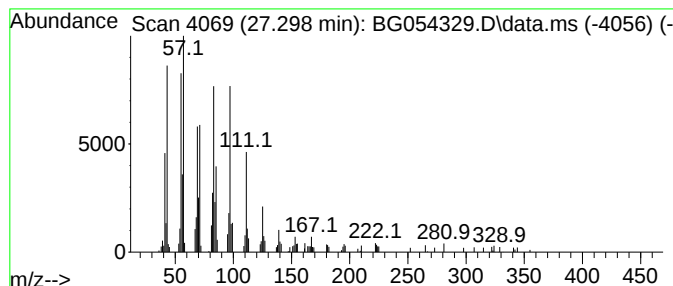
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.298	9.20 ng	392139	Perylene-d12	24.836

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	95
2			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	95
3			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	95
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	95
5			Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	95



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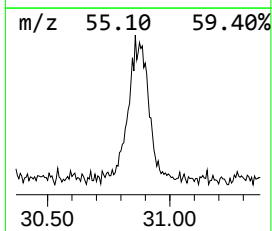
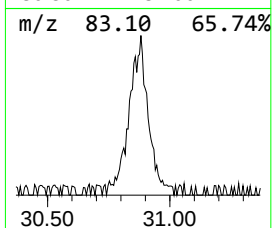
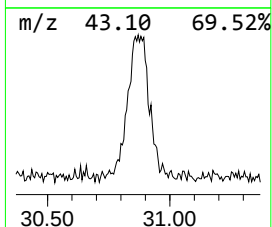
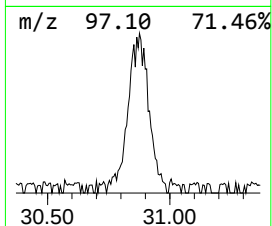
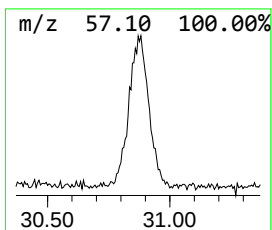
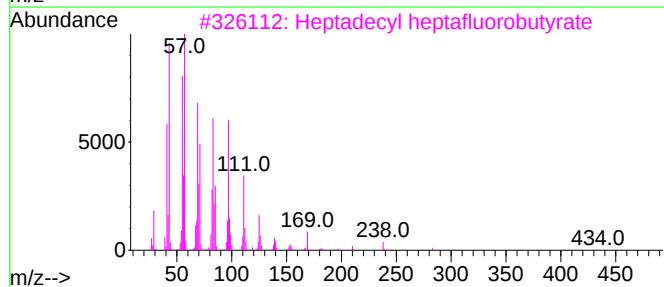
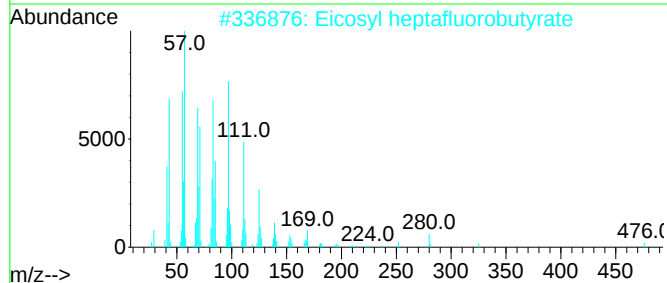
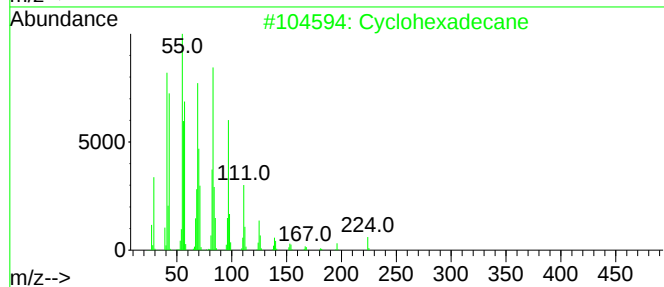
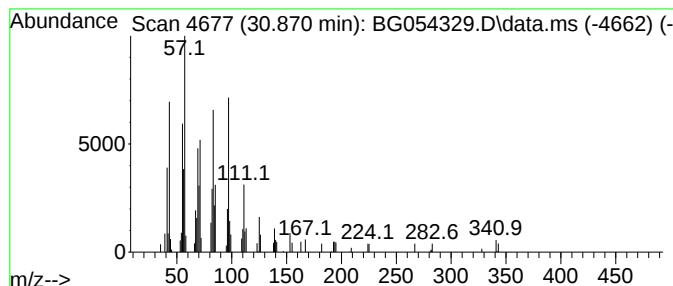
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.870	5.32 ng	226803	Perylene-d12	24.836

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	90
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4			17-Pentatriacontene	491	C35H70	006971-40-0	90
5			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054329.D
Acq On : 20 Jul 2022 15:58
Operator : CG/JU
Sample : N3771-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-7F

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Ethanol, 2-(2-b...	10.565	3.5	ng	24650	2	10.800	139582	20.0
Tridecanoic acid	18.267	2.8	ng	44932	4	17.374	324433	20.0
unknown21.405	21.405	2.2	ng	48062	5	21.640	429751	20.0
1-Hexacosene	23.097	5.4	ng	116082	5	21.640	429751	20.0
Tricosyl triflu...	27.298	9.2	ng	392139	6	24.836	852928	20.0
Cyclohexadecane	30.870	5.3	ng	226803	6	24.836	852928	20.0