

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032723\
 Data File : BP014332.D
 Acq On : 28 Mar 2023 02:17
 Operator : CG/JU
 Sample : 02055-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-2

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_P\Methods\8270E-BP030623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP014332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.105	317	326	340	rBV	336701	504037	3.28%	0.997%
2	5.569	399	405	422	rBV	1156496	1777944	11.56%	3.515%
3	7.187	673	680	694	rBV	596887	1075171	6.99%	2.126%
4	8.022	812	822	835	rBV	444739	717518	4.67%	1.419%
5	9.199	1014	1022	1042	rBV	1603864	2768143	18.00%	5.473%
6	10.846	1295	1302	1318	rBV	520971	947483	6.16%	1.873%
7	13.293	1711	1718	1736	rBV	4202449	6018321	39.13%	11.899%
8	14.669	1944	1952	1966	rBV	768810	1213457	7.89%	2.399%
9	16.163	2199	2206	2228	rBV	3238444	4804358	31.24%	9.499%
10	17.428	2415	2421	2435	rBV	1021597	1519953	9.88%	3.005%
11	18.292	2563	2568	2589	rBV	597046	1118593	7.27%	2.212%
12	19.516	2772	2776	2789	rBV	210200	418756	2.72%	0.828%
13	19.969	2848	2853	2865	rBV	6597793	7897367	51.35%	15.614%
14	21.198	3058	3062	3072	rBV3	201534	424901	2.76%	0.840%
15	21.510	3110	3115	3121	rBV	1318808	1823235	11.85%	3.605%
16	21.633	3130	3136	3155	rBV	10126757	15379732	100.00%	30.408%
17	22.774	3327	3330	3336	rVB2	145880	202857	1.32%	0.401%
18	24.027	3536	3543	3554	rVB2	895932	1966827	12.79%	3.889%

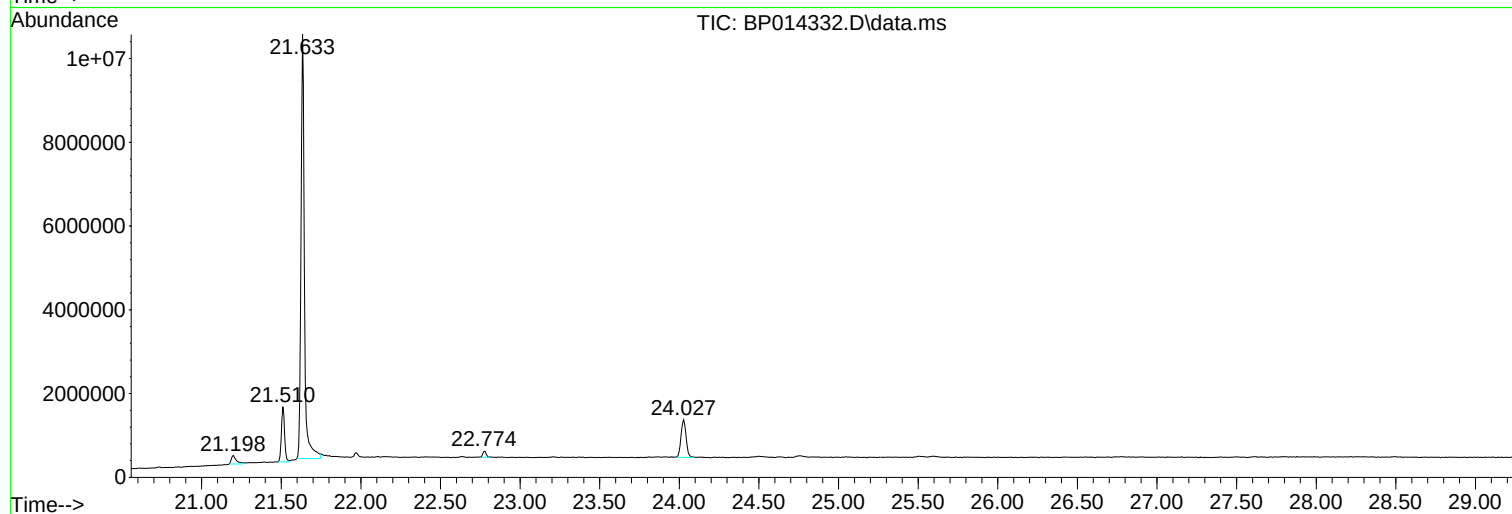
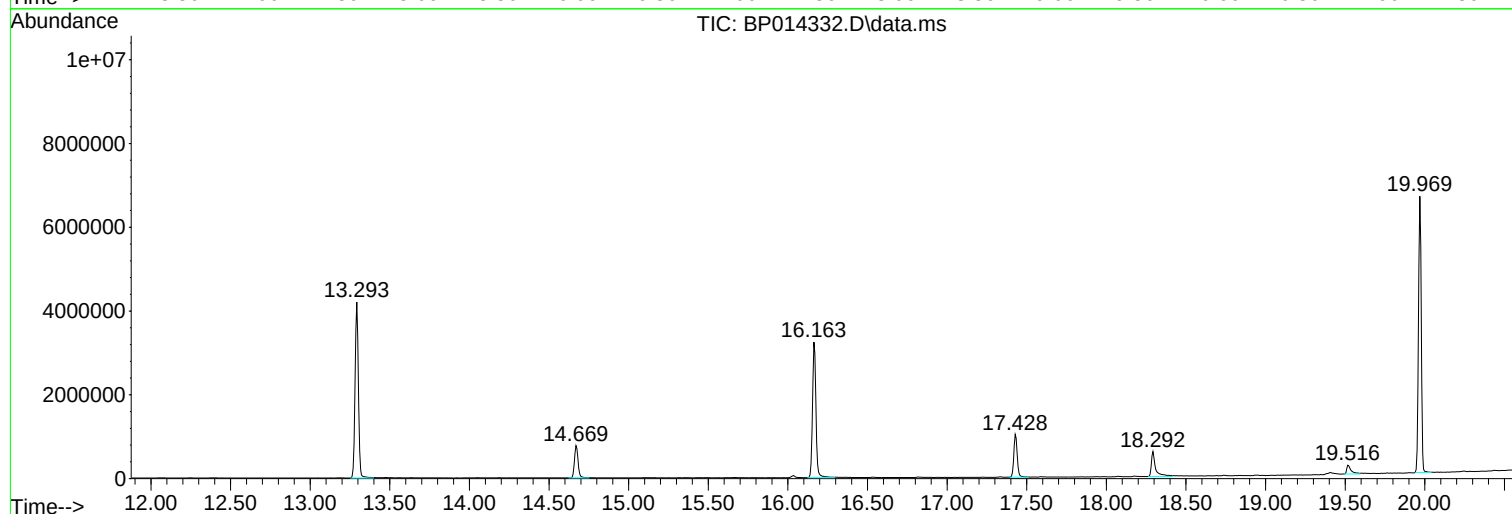
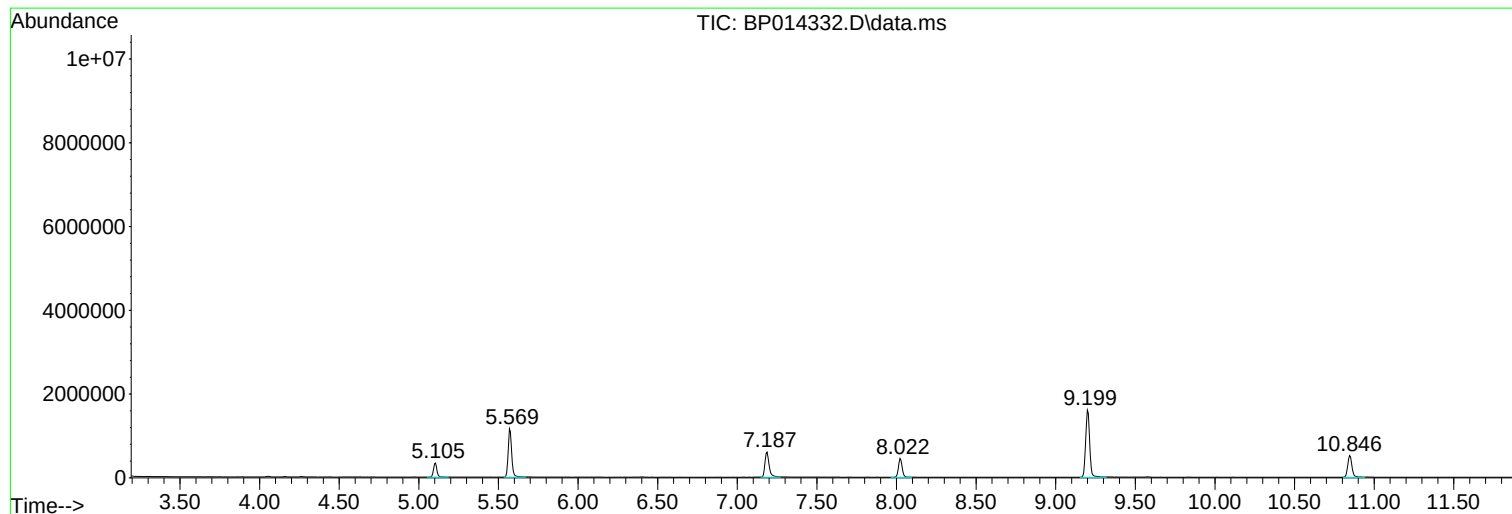
Sum of corrected areas: 50578653

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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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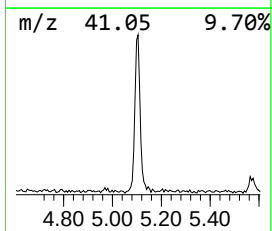
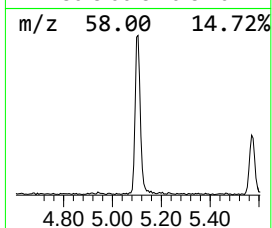
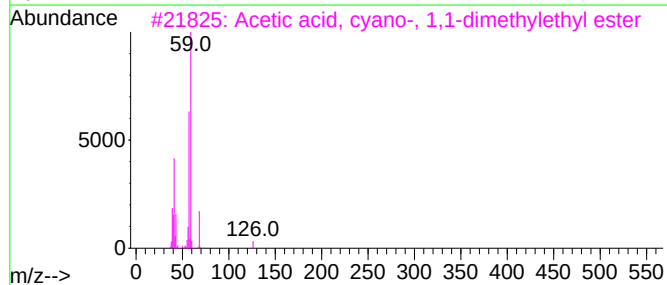
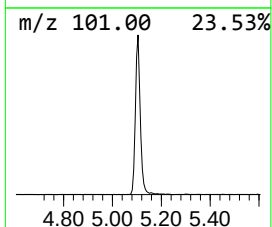
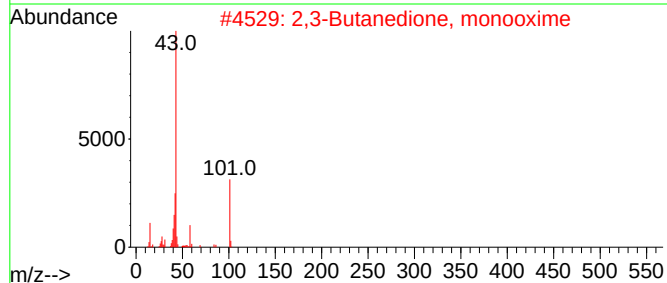
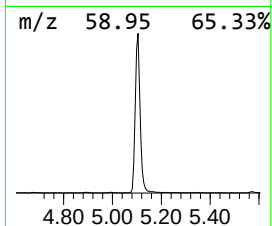
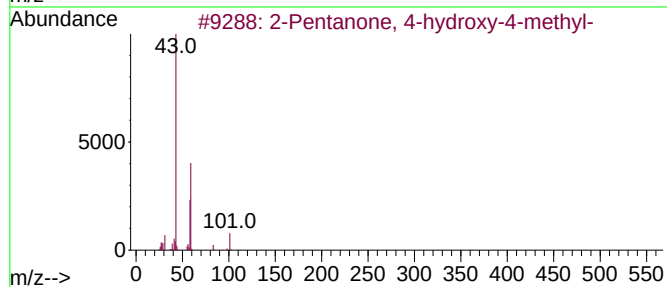
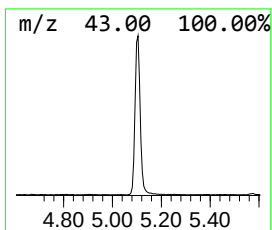
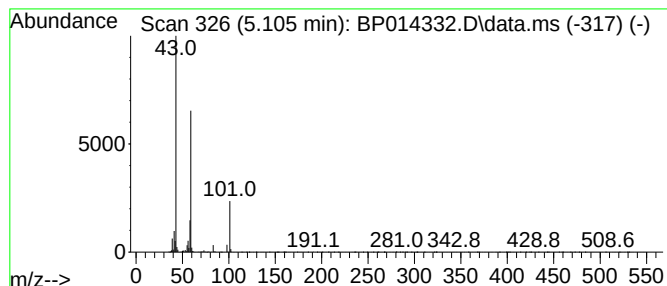
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.105	14.05 ng	504037	1,4-Dichlorobenzene-d4	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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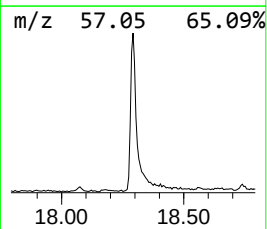
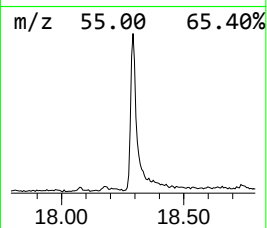
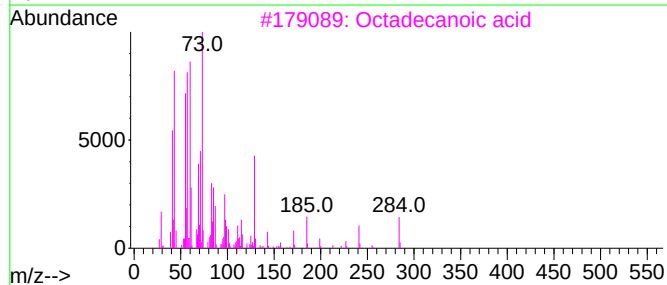
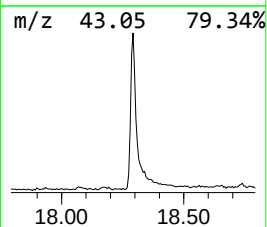
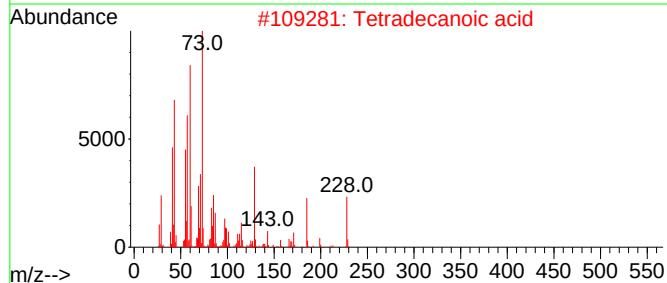
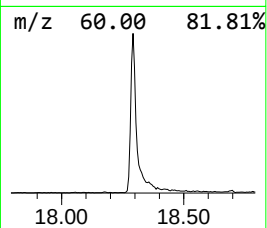
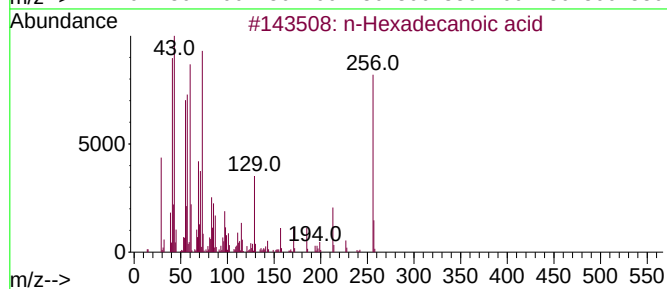
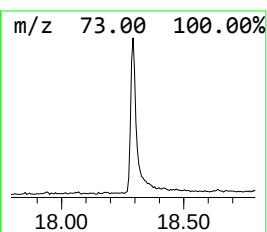
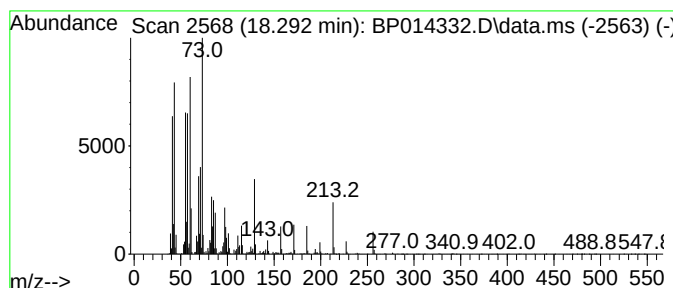
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.292	14.72 ng	1118590	Phenanthrene-d10	17.428	
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	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87



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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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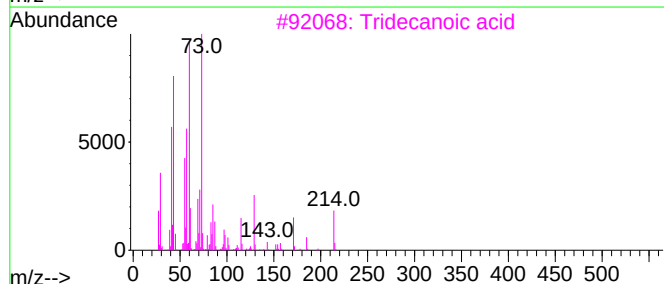
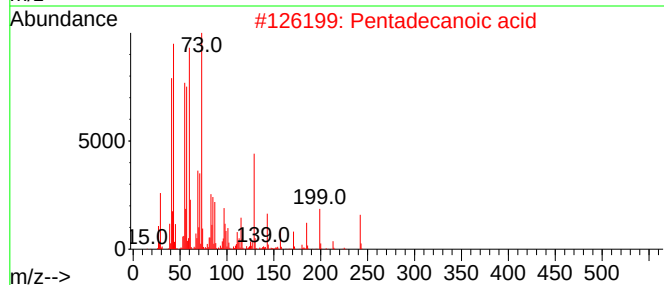
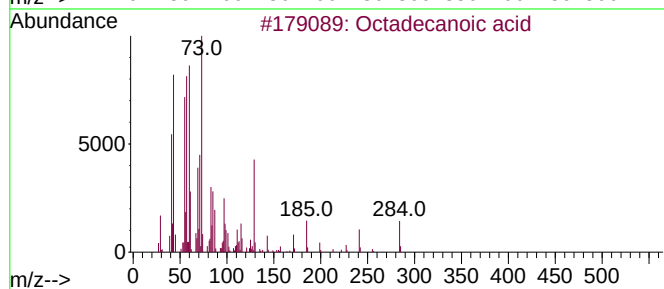
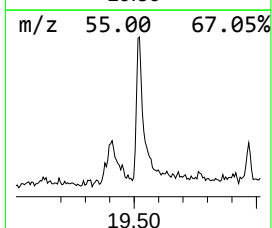
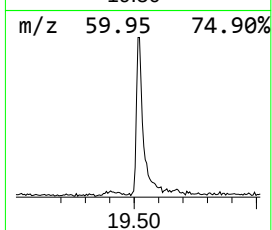
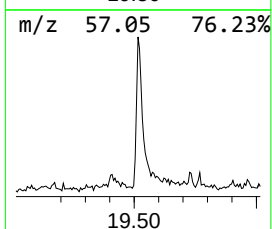
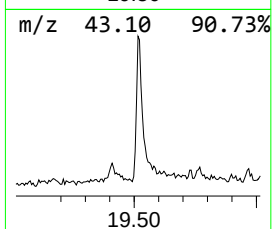
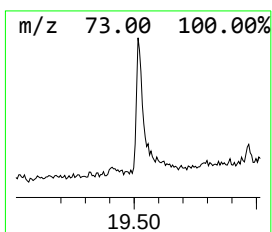
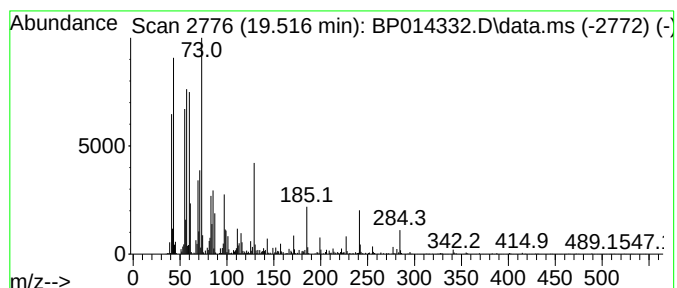
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.516	4.59 ng	418756	Chrysene-d12	21.510

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	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	70
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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Instrument :
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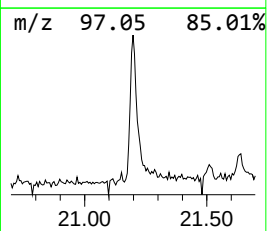
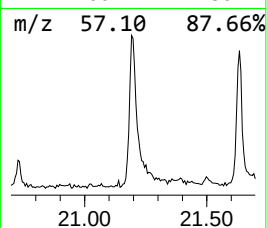
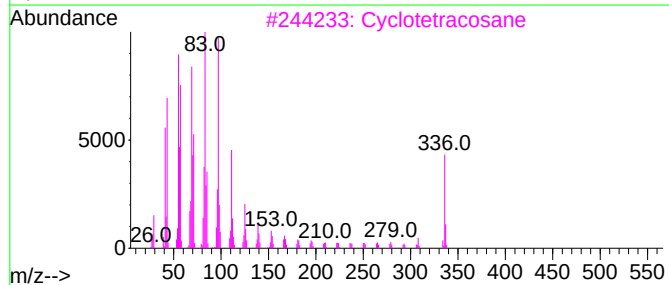
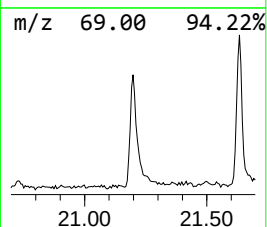
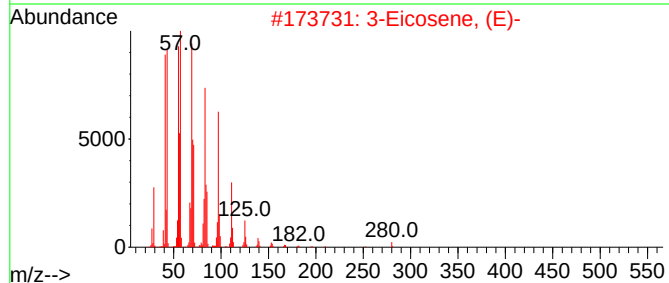
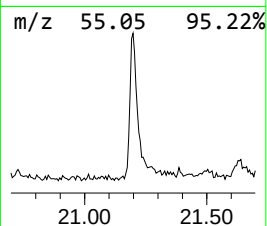
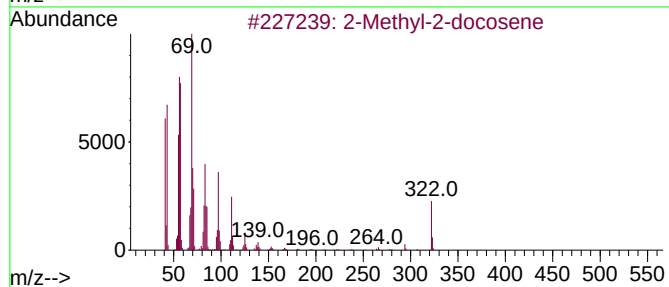
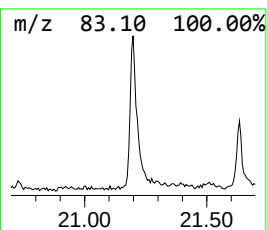
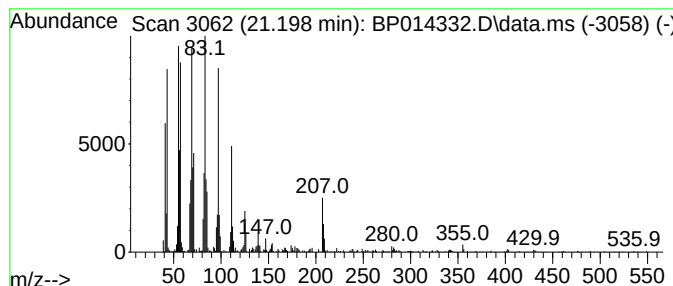
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Peak Number 4 2-Methyl-2-docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	4.66 ng	424901	Chrysene-d12	21.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-2-docosene	322	C23H46	1000131-16-9	97
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3			Cyclotetracosane	336	C24H48	000297-03-0	95
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
5			1-Tricosene	322	C23H46	018835-32-0	95



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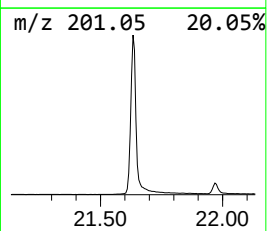
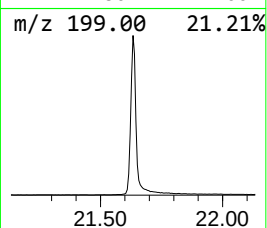
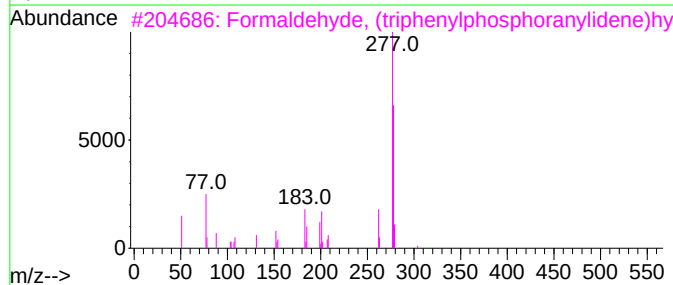
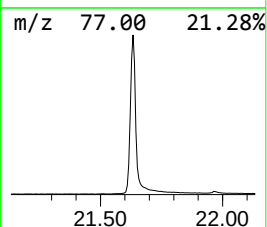
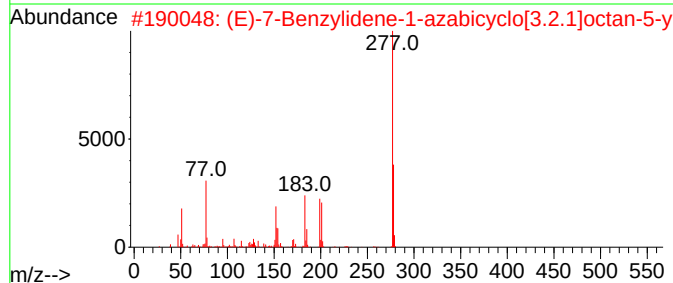
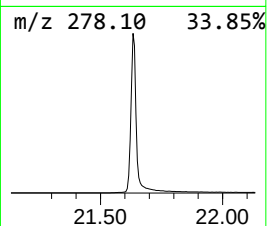
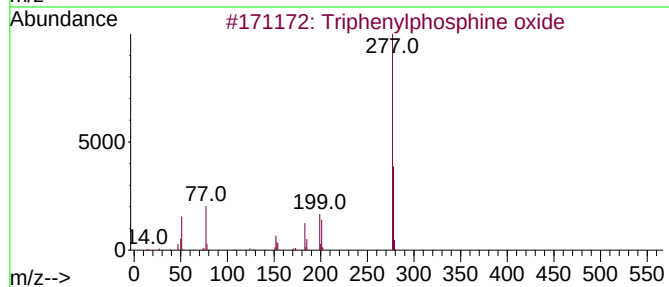
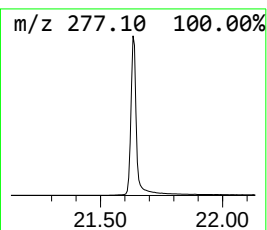
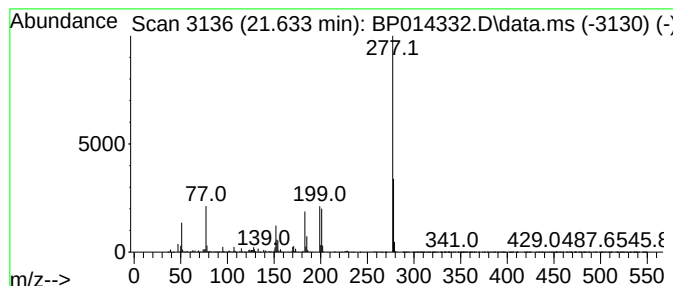
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.633	168.71 ng	15379700	Chrysene-d12	21.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	17



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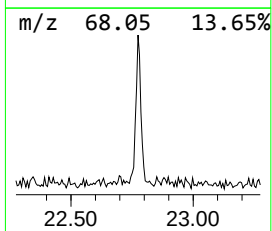
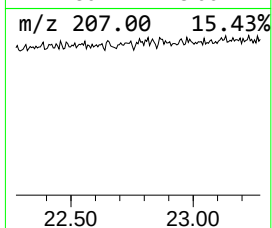
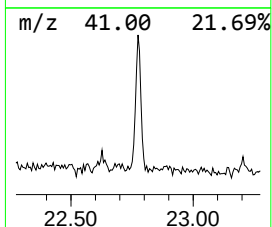
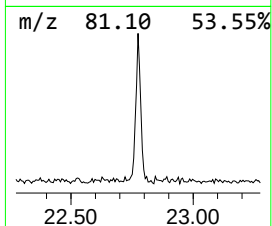
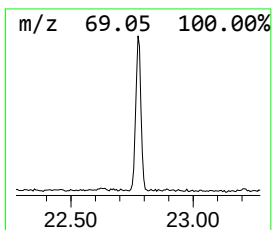
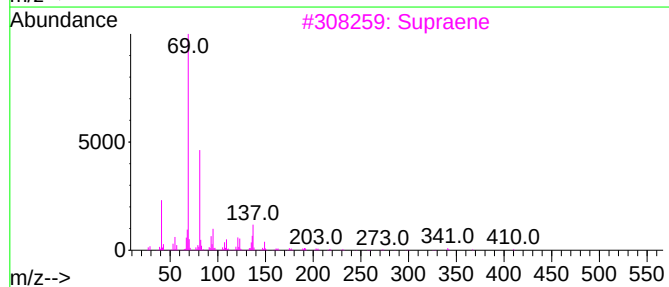
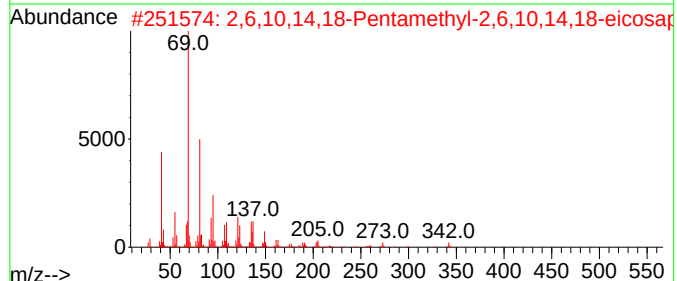
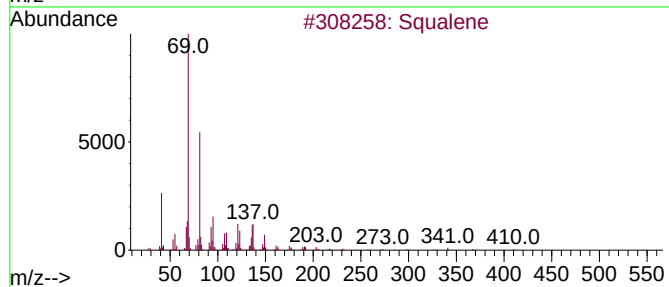
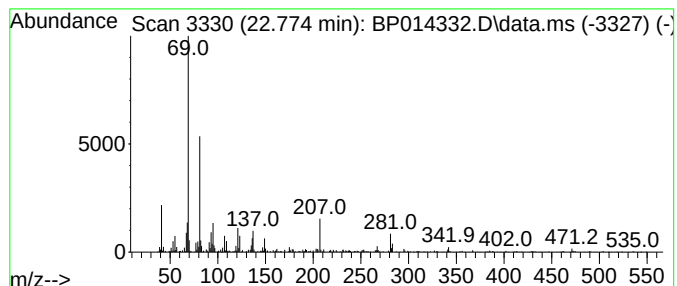
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.774	2.06 ng	202857	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	76
3			Supraene	410	C30H50	007683-64-9	68
4			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	64
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032723\
Data File : BP014332.D
Acq On : 28 Mar 2023 02:17
Operator : CG/JU
Sample : 02055-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030623.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
2-Pentanone, 4-...	5.105	14.1	ng	504037	1	8.022	717518	20.0
n-Hexadecanoic ...	18.292	14.7	ng	1118590	4	17.428	1519950	20.0
Octadecanoic acid	19.516	4.6	ng	418756	5	21.510	1823240	20.0
2-Methyl-2-doco...	21.198	4.7	ng	424901	5	21.510	1823240	20.0
Triphenylphosph...	21.633	168.7	ng	15379700	5	21.510	1823240	20.0
Squalene	22.774	2.1	ng	202857	6	24.027	1966830	20.0