

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
 Data File : BM035165.D
 Acq On : 19 May 2022 22:47
 Operator : CG/JU
 Sample : N2871-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P017-SS001-0006-01

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-BM042722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035165.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	323	328	334	rBV	68759	102850	1.48%	0.230%
2	5.481	400	407	416	rBV	2530468	3586474	51.75%	8.022%
3	7.075	670	678	688	rBV	2358248	3665834	52.90%	8.200%
4	7.904	811	819	826	rBV	556608	859581	12.40%	1.923%
5	9.063	1007	1016	1031	rBV	1432672	2369824	34.20%	5.301%
6	10.704	1288	1295	1303	rBV	693672	1145895	16.54%	2.563%
7	13.169	1707	1714	1728	rBV	3435598	4978244	71.84%	11.135%
8	13.998	1850	1855	1860	rBV	62228	95144	1.37%	0.213%
9	14.539	1941	1947	1955	rBV	988181	1479560	21.35%	3.309%
10	16.027	2194	2200	2217	rBV	2852651	3935789	56.79%	8.804%
11	16.210	2226	2231	2235	rVB	64012	76667	1.11%	0.171%
12	17.186	2391	2397	2400	rBV	90656	125766	1.81%	0.281%
13	17.286	2405	2414	2420	rVV	1187955	1715978	24.76%	3.838%
14	17.345	2420	2424	2427	rVV	68270	93764	1.35%	0.210%
15	17.386	2427	2431	2439	rVB3	36385	76281	1.10%	0.171%
16	18.127	2552	2557	2562	rBV	93114	131059	1.89%	0.293%
17	18.192	2562	2568	2578	rBV	781356	1100549	15.88%	2.462%
18	18.486	2614	2618	2626	rBV	60468	102884	1.48%	0.230%
19	19.321	2756	2760	2761	rBV2	71935	86479	1.25%	0.193%
20	19.345	2761	2764	2766	rBV2	108770	119742	1.73%	0.268%
21	19.462	2780	2784	2801	rBV	322604	522371	7.54%	1.168%
22	19.721	2824	2828	2840	rBV2	312668	425872	6.15%	0.953%
23	19.909	2855	2860	2866	rVB	5959068	6929900	100.00%	15.501%
24	21.186	3073	3077	3084	rVB	712812	914584	13.20%	2.046%
25	21.386	3108	3111	3116	rBV	265598	294346	4.25%	0.658%
26	21.468	3120	3125	3132	rVB	1575960	2045884	29.52%	4.576%
27	22.092	3228	3231	3242	rBV3	167387	344204	4.97%	0.770%
28	23.850	3524	3530	3539	rVB2	1032509	2066127	29.81%	4.622%
29	24.574	3648	3653	3668	rVB	320391	777870	11.22%	1.740%
30	25.815	3859	3864	3875	rVB2	367807	924850	13.35%	2.069%
31	26.462	3968	3974	3984	rVB	370556	985961	14.23%	2.205%
32	28.744	4355	4362	4376	rVB4	760445	2626170	37.90%	5.874%

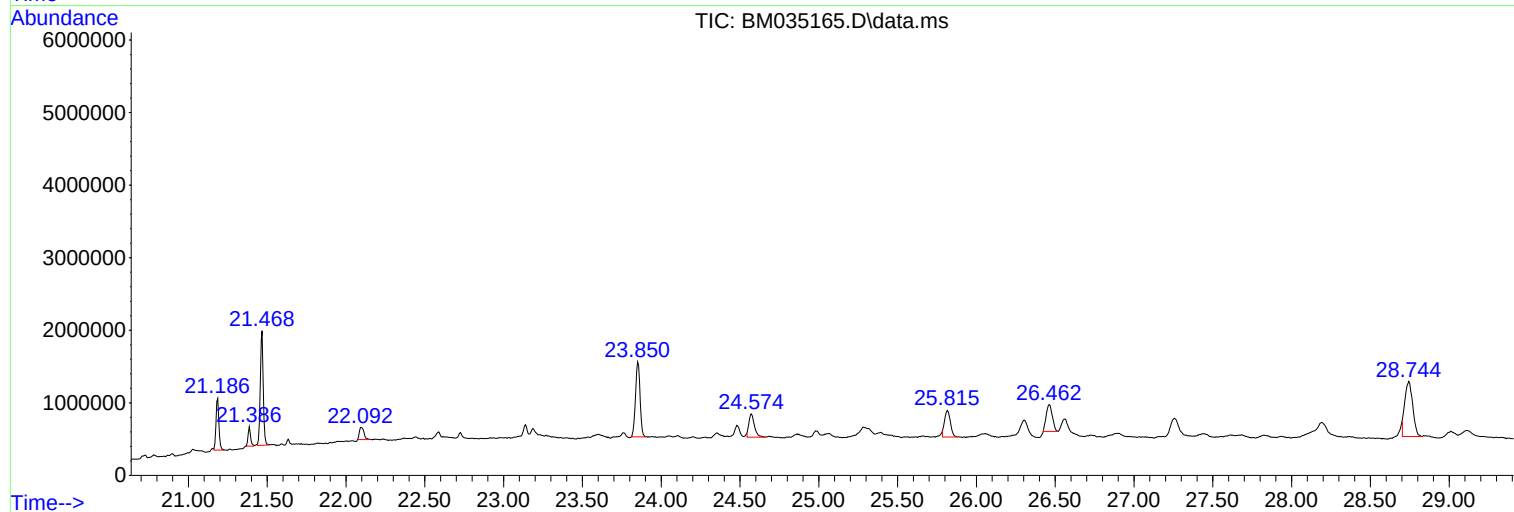
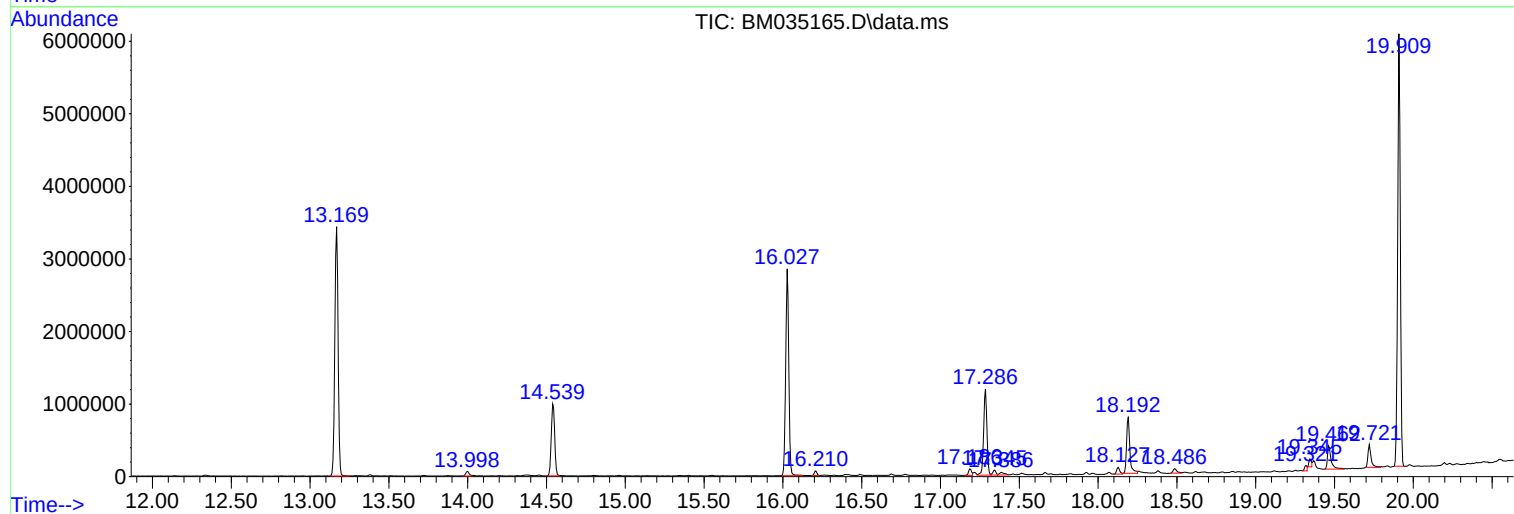
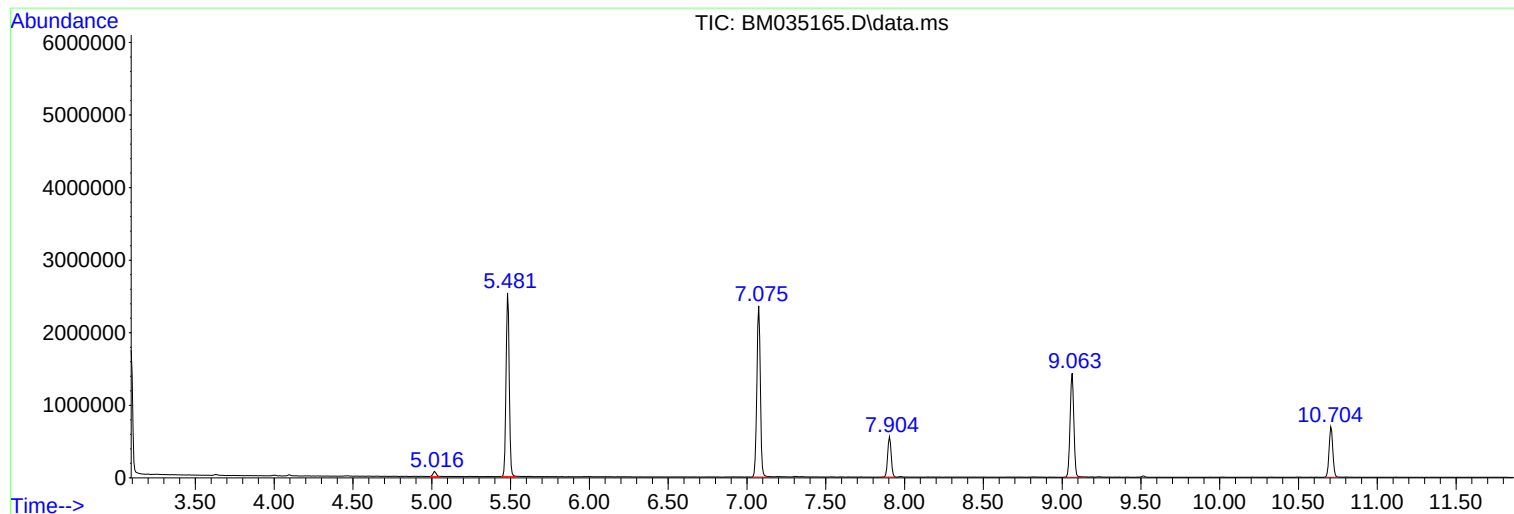
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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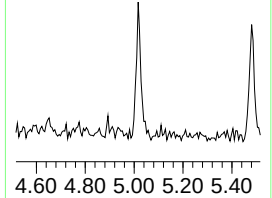
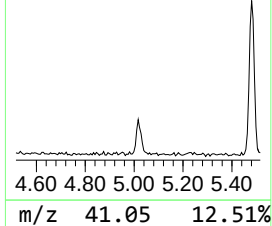
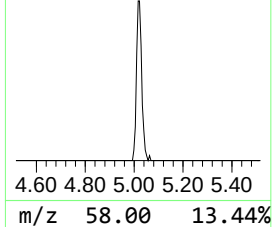
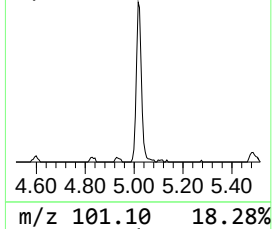
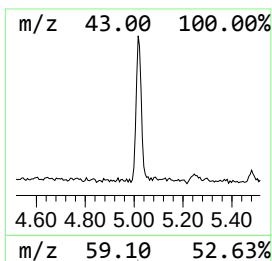
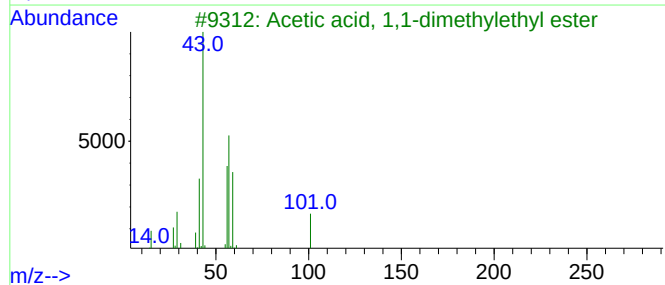
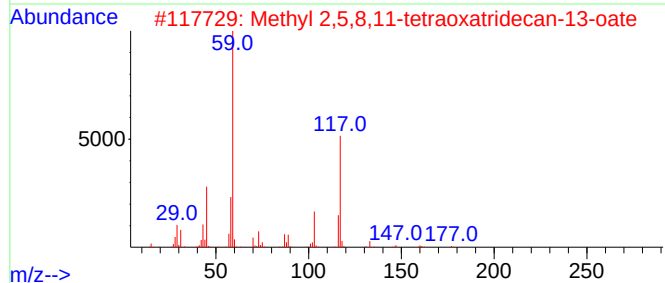
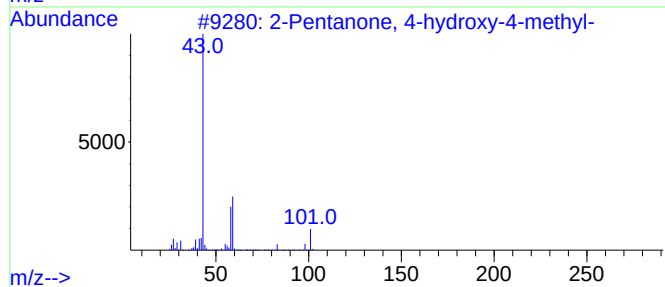
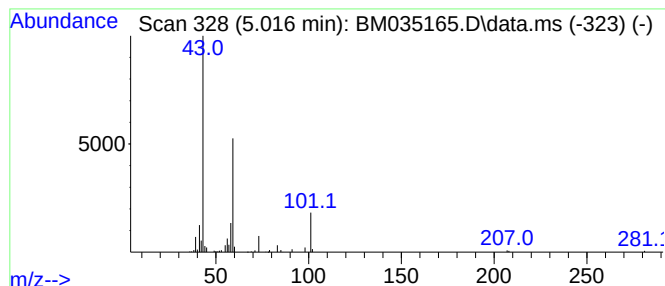
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.39 ng	102850	1,4-Dichlorobenzene-d4	7.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	47		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
4	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	36		
5	Methyl 2,5,8,11,14,17-hexaoxanon...	324	C14H28O8	1000366-81-4	33		



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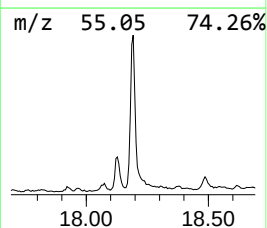
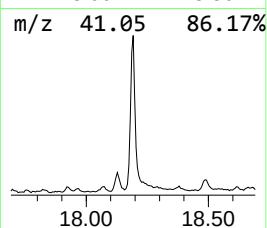
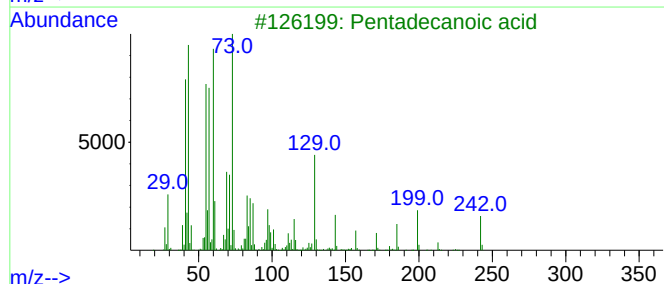
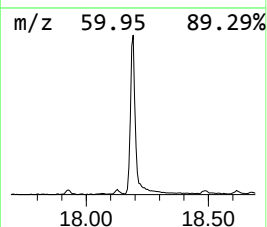
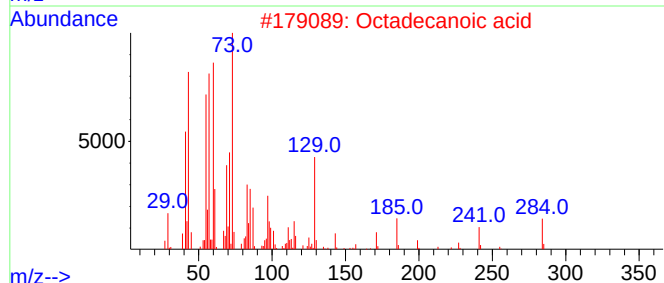
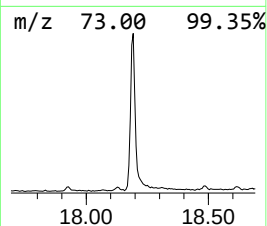
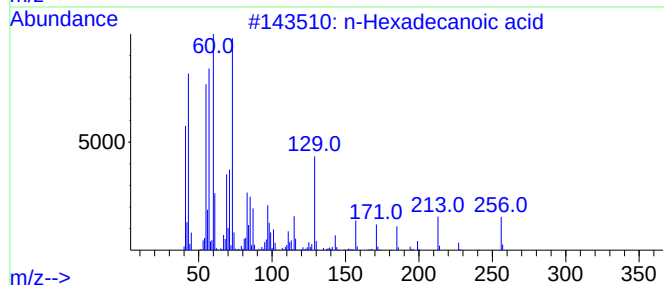
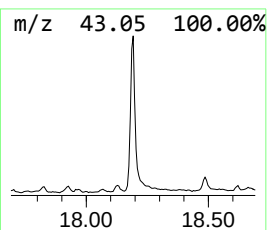
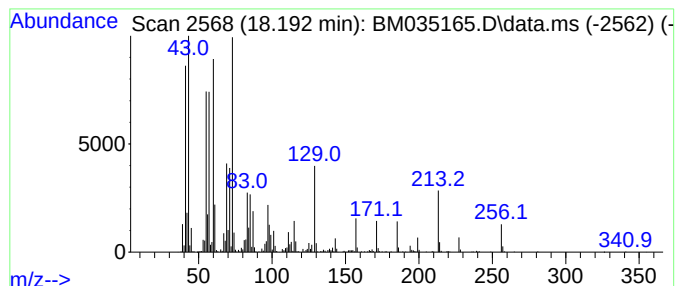
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	12.83 ng	1100550	Phenanthrene-d10	17.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	62



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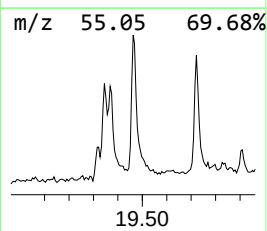
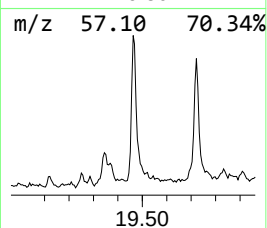
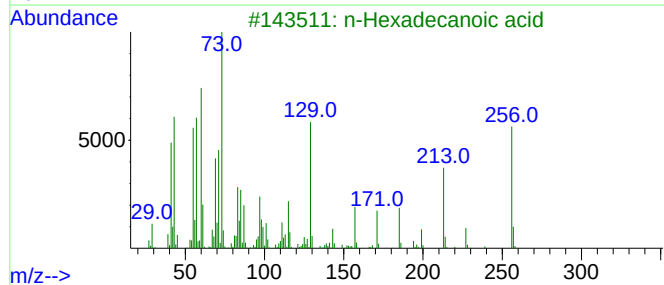
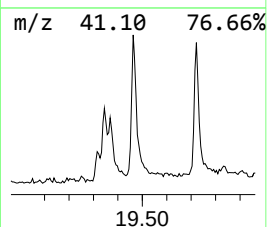
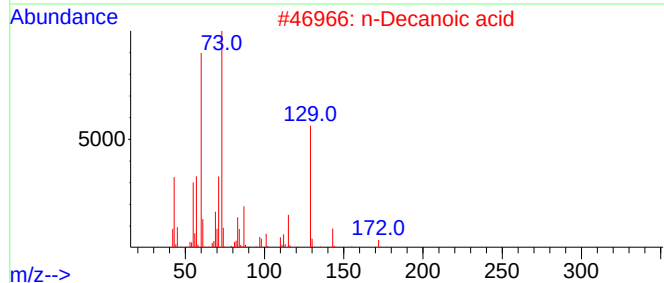
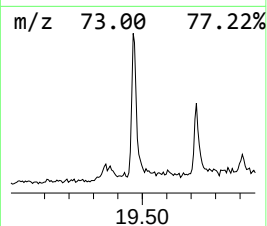
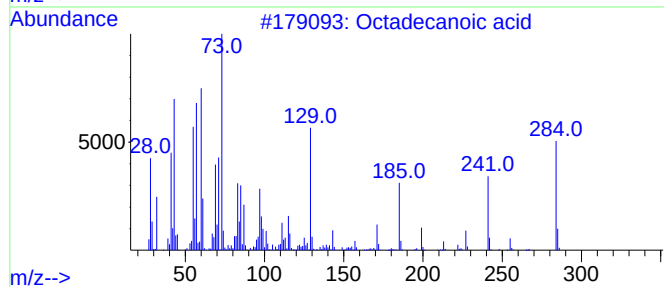
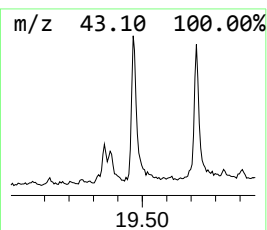
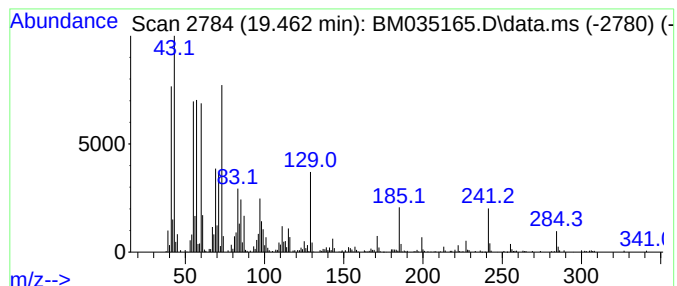
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	5.11 ng	522371	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	70



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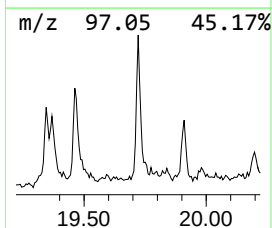
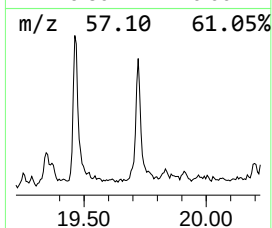
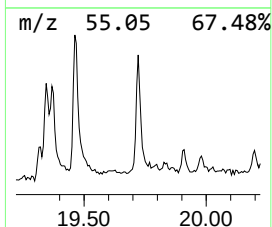
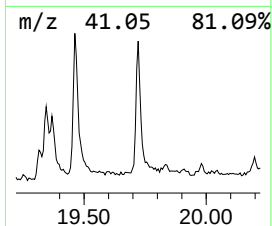
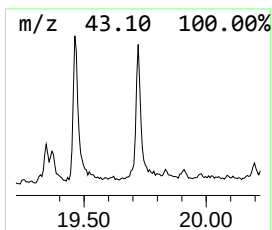
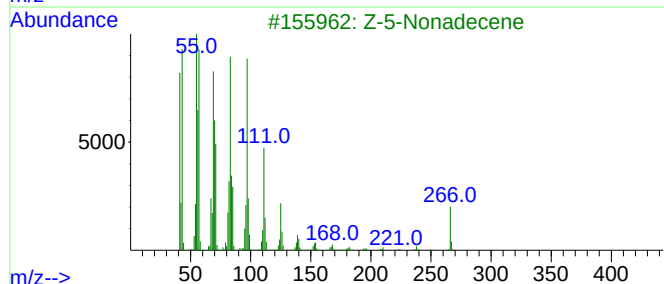
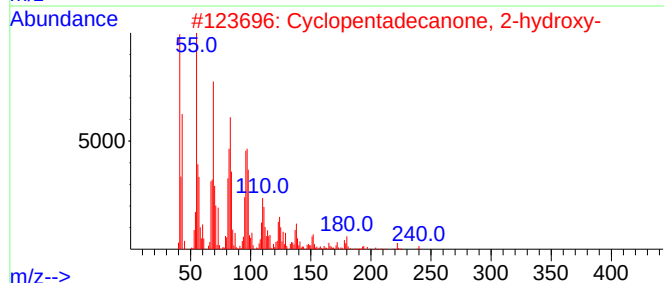
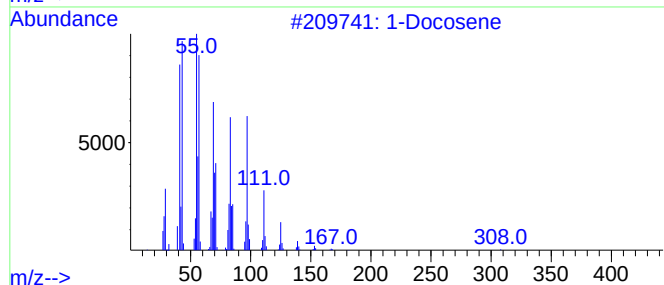
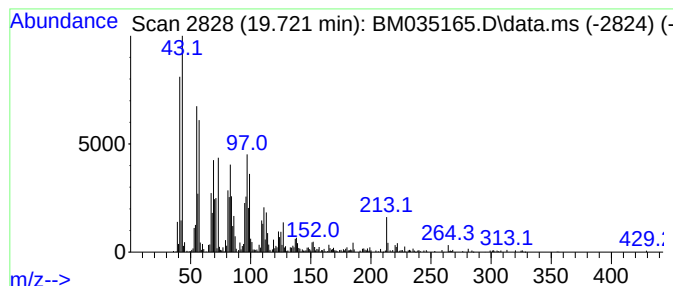
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Peak Number 4 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.721	4.16 ng	425872	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	96
2			Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	92
3			Z-5-Nonadecene	266	C19H38	1000131-11-8	90
4			Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	86
5			Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	84



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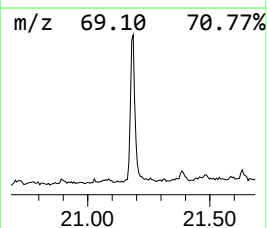
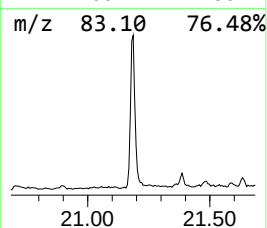
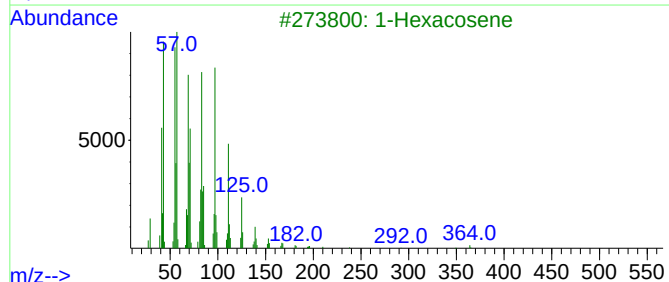
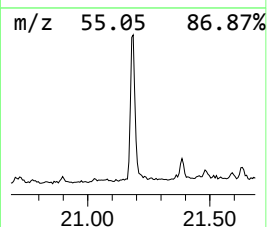
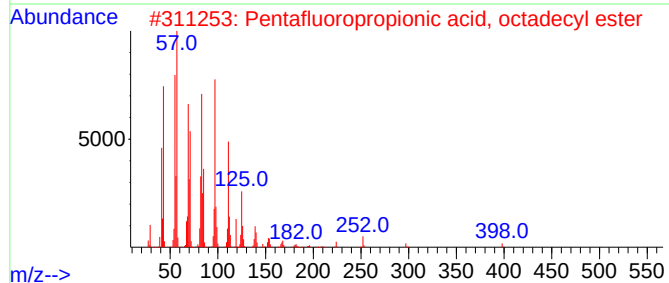
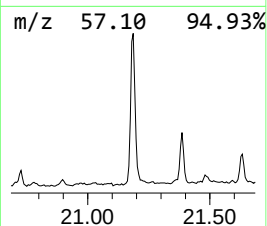
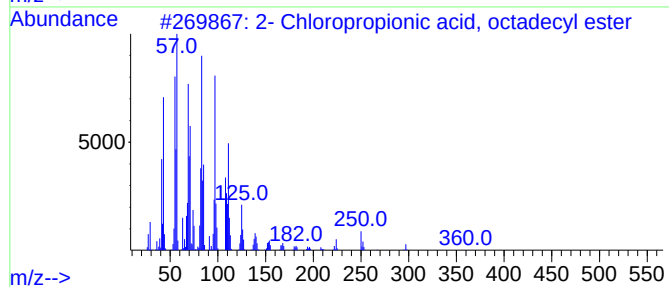
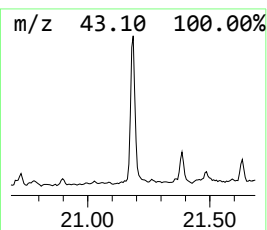
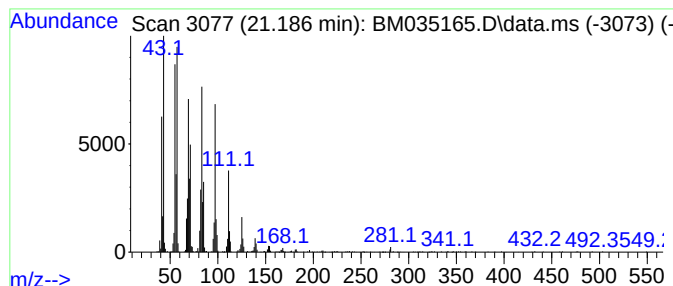
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Peak Number 5 2- Chloropropionic acid, oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	8.94 ng	914584	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	96	
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	94		
3	1-Hexacosene	364	C26H52	018835-33-1	94		
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94		
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94		



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P017-SS001-0006-01

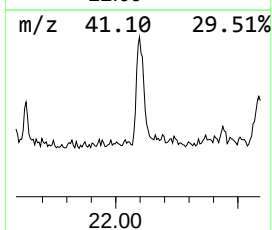
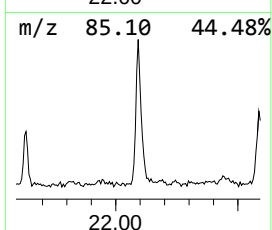
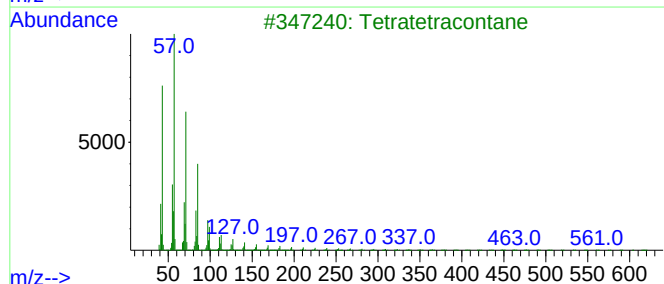
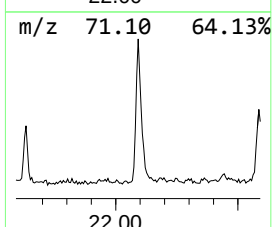
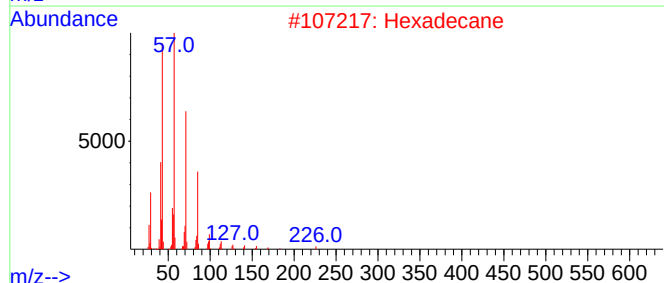
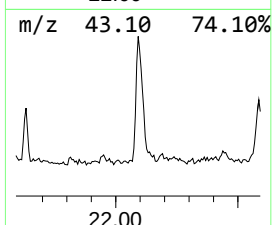
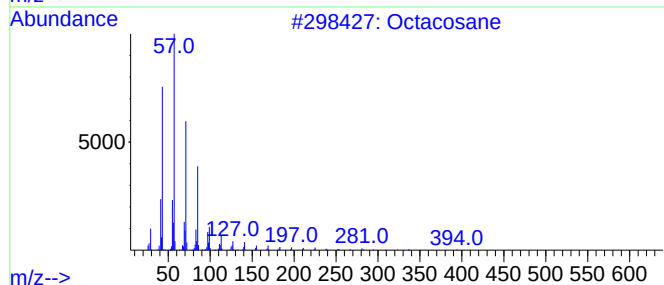
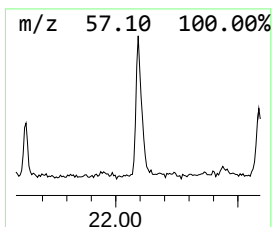
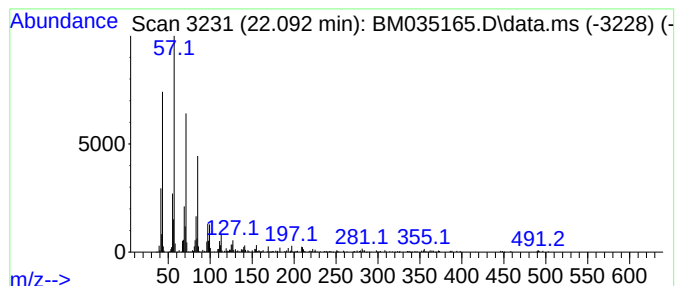
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.092	3.36 ng	344204	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	99
2			Hexadecane	226	C16H34	000544-76-3	93
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035165.D
Acq On : 19 May 2022 22:47
Operator : CG/JU
Sample : N2871-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P017-SS001-0006-01

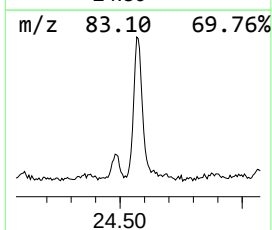
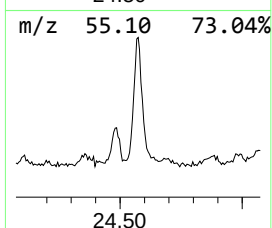
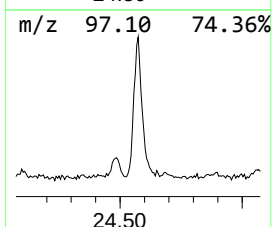
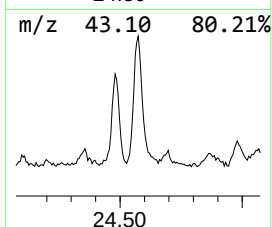
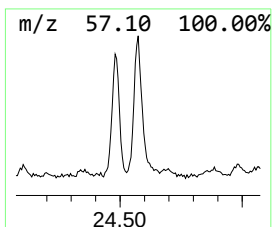
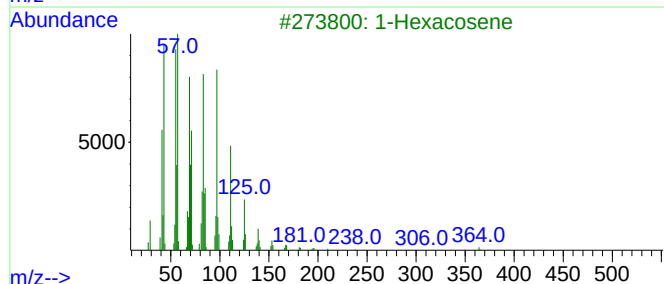
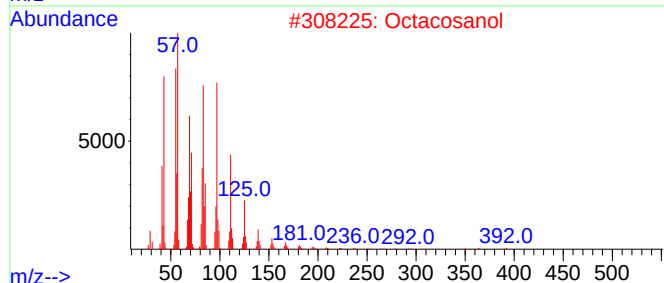
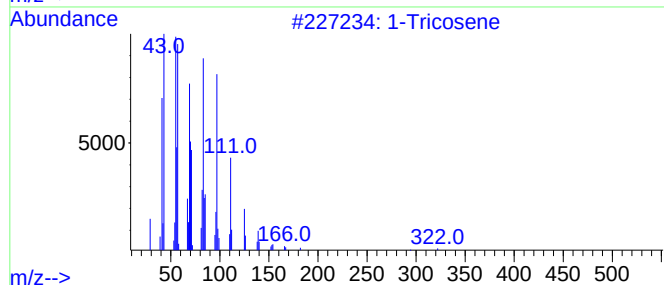
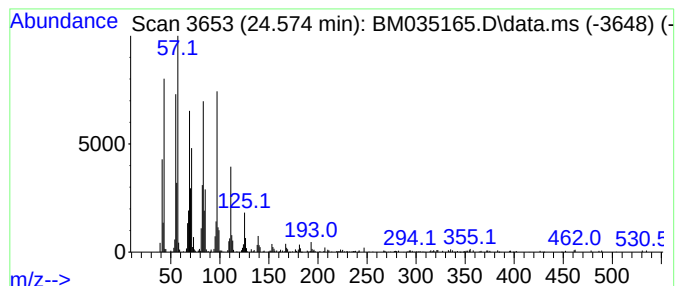
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.574	7.53 ng	777870	Perylene-d12	23.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tricosene	322	C23H46	018835-32-0	95
2			Octacosanol	410	C28H58O	000557-61-9	95
3			1-Hexacosene	364	C26H52	018835-33-1	95
4			1-Heptacosanol	396	C27H56O	002004-39-9	93
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035165.D
Acq On : 19 May 2022 22:47
Operator : CG/JU
Sample : N2871-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P017-SS001-0006-01

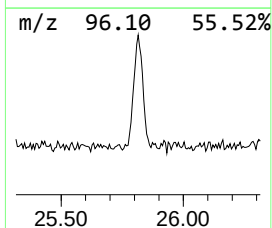
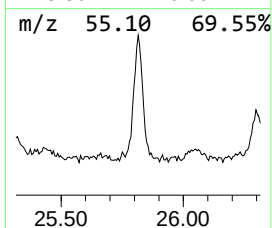
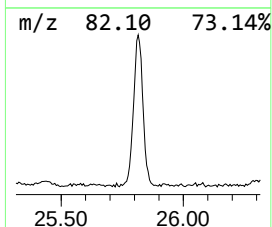
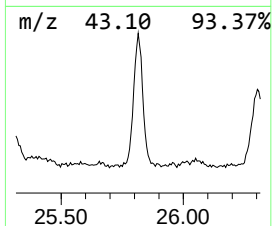
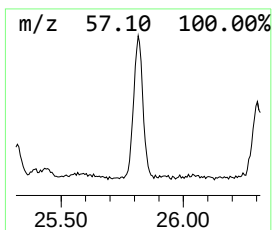
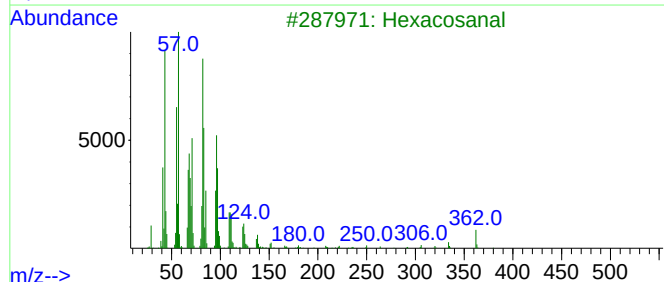
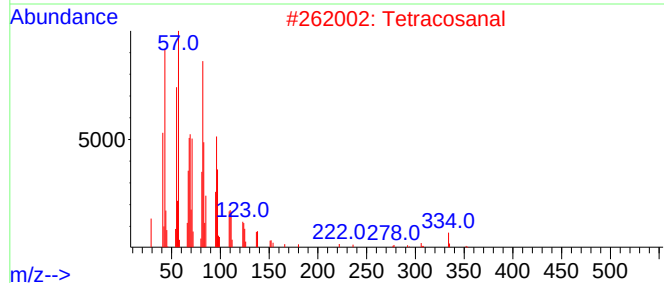
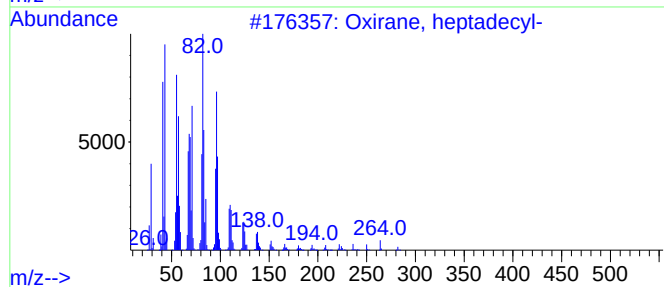
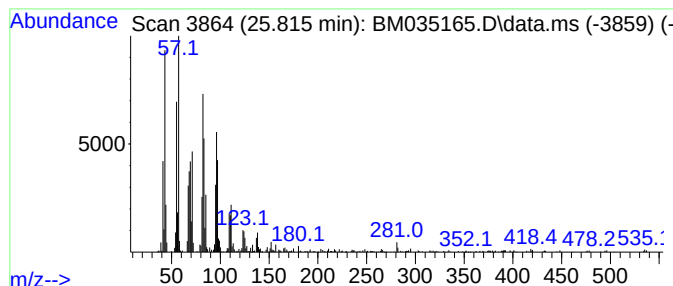
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.815	8.95 ng	924850	Perylene-d12	23.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2			Tetracosanal	352	C24H48O	057866-08-7	91
3			Hexacosanal	380	C26H52O	026627-85-0	91
4			Octadecanal	268	C18H36O	000638-66-4	91
5			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035165.D
Acq On : 19 May 2022 22:47
Operator : CG/JU
Sample : N2871-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P017-SS001-0006-01

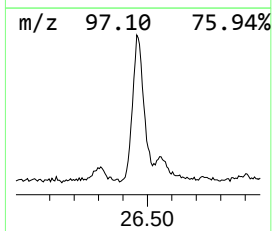
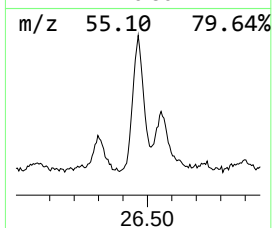
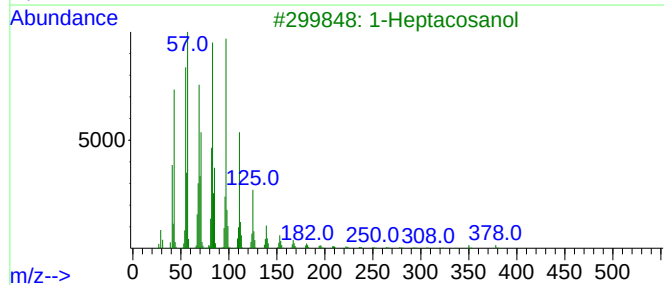
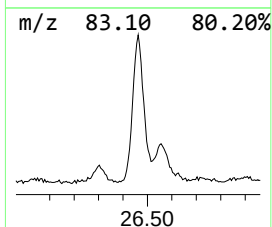
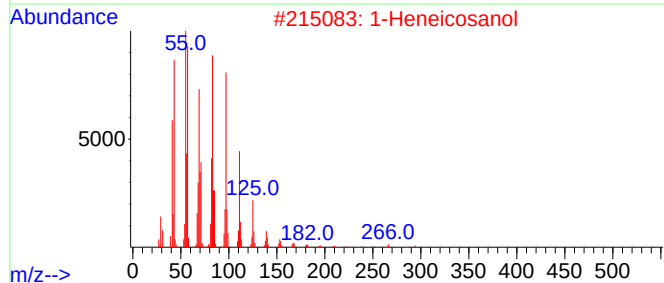
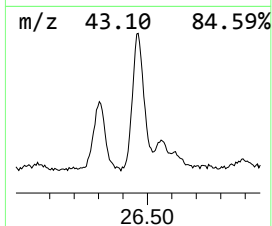
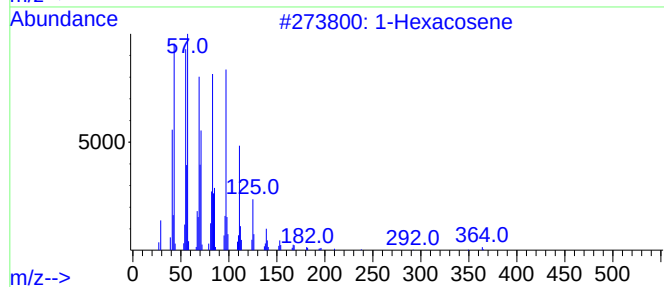
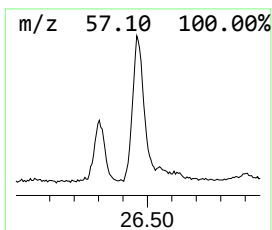
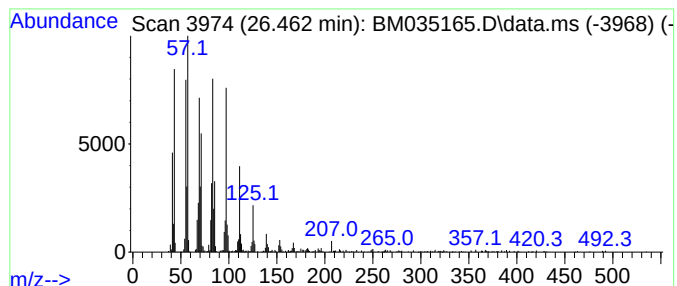
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.462	9.54 ng	985961	Perylene-d12	23.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	1-Heneicosanol			312	C21H44O	015594-90-8	93
3	1-Heptacosanol			396	C27H56O	002004-39-9	93
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	93
5	Heptacosyl acetate			438	C29H58O2	1000351-78-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035165.D
Acq On : 19 May 2022 22:47
Operator : CG/JU
Sample : N2871-01
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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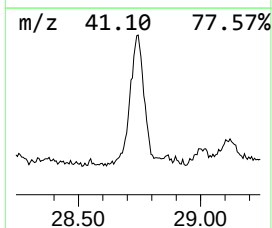
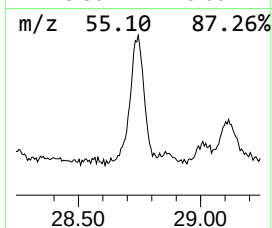
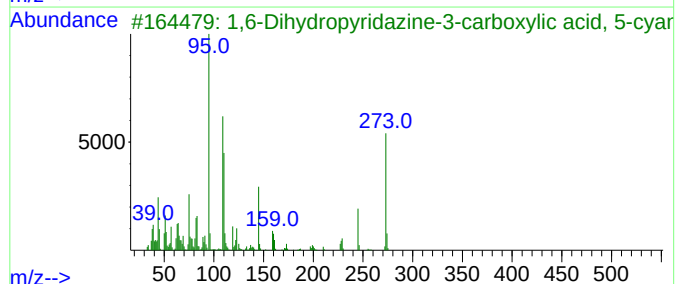
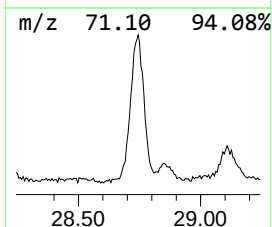
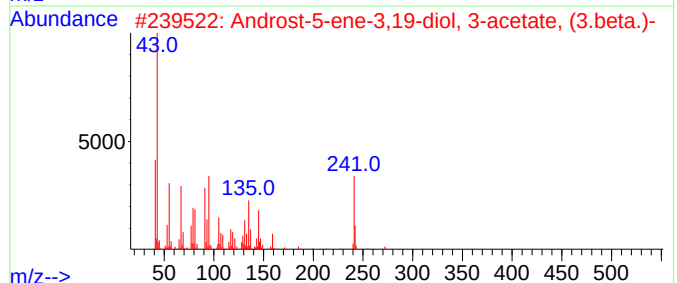
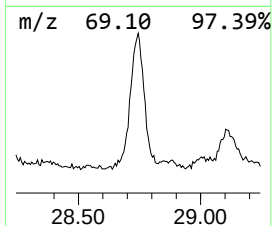
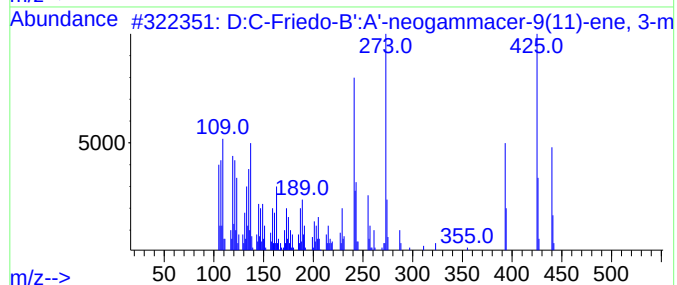
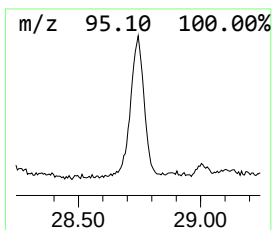
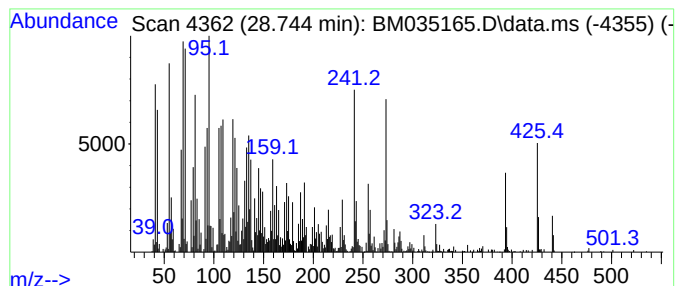
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.744	25.42 ng	2626170	Perylene-d12	23.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	64
2			Androst-5-ene-3,19-diol, 3-aceta...	332	C21H32O3	055320-48-4	38
3			1,6-Dihydropyridazine-3-carboxyl...	273	C13H8FN3O3	1000304-05-0	30
4			3H-Thiazolo[4,5-d]pyrimidine-2-t...	241	C9H11N3OS2	1000304-97-8	25
5			2,3,6,7-Tetrahydro-1H,5H,11H-pyr...	241	C15H15NO2	058336-35-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035165.D
Acq On : 19 May 2022 22:47
Operator : CG/JU
Sample : N2871-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P017-SS001-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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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n-Hexadecanoic ...	18.192	12.8	ng	1100550	4	17.286	1715980	20.0
Octadecanoic acid	19.462	5.1	ng	522371	5	21.468	2045880	20.0
1-Docosene	19.721	4.2	ng	425872	5	21.468	2045880	20.0
2-Chloropropio...	21.186	8.9	ng	914584	5	21.468	2045880	20.0
Octacosane	22.092	3.4	ng	344204	5	21.468	2045880	20.0
1-Tricosene	24.574	7.5	ng	777870	6	23.850	2066130	20.0
Oxirane, heptad...	25.815	8.9	ng	924850	6	23.850	2066130	20.0
1-Hexacosene	26.462	9.5	ng	985961	6	23.850	2066130	20.0
D:C-Friedo-B':A...	28.744	25.4	ng	2626170	6	23.850	2066130	20.0