

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
 Data File : BM041207.D
 Acq On : 01 Aug 2023 03:18
 Operator : MA/JU
 Sample : 03741-13
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P6B

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.881	112	118	124	rBV	41030	68227	1.47%	0.155%
2	5.369	364	371	387	rBV	1916598	2743279	59.04%	6.222%
3	6.975	637	644	662	rBV	1824316	2843949	61.20%	6.450%
4	7.798	777	784	792	rBV	706852	1092540	23.51%	2.478%
5	8.969	974	983	998	rBV	1065906	1781748	38.34%	4.041%
6	10.604	1248	1261	1268	rBV	882426	1462480	31.47%	3.317%
7	13.080	1674	1682	1701	rBV	2584875	3662063	78.81%	8.305%
8	13.927	1819	1826	1838	rBV	138276	208888	4.50%	0.474%
9	14.463	1910	1917	1924	rBV	1221444	1733895	37.31%	3.932%
10	15.045	2007	2016	2029	rBV2	54286	218155	4.69%	0.495%
11	15.963	2163	2172	2180	rBV	2167952	2987339	64.29%	6.775%
12	16.186	2204	2210	2217	rBV5	28102	68896	1.48%	0.156%
13	16.968	2337	2343	2346	rBV	35668	58454	1.26%	0.133%
14	17.221	2380	2386	2391	rBV	1440939	2015053	43.37%	4.570%
15	17.262	2391	2393	2397	rVB	72590	83716	1.80%	0.190%
16	18.121	2532	2539	2549	rBV2	426159	770610	16.58%	1.748%
17	18.292	2563	2568	2572	rBV2	76200	133908	2.88%	0.304%
18	19.021	2688	2692	2698	rBV2	84049	159755	3.44%	0.362%
19	19.115	2706	2708	2712	rVB2	48322	51267	1.10%	0.116%
20	19.180	2714	2719	2729	rVB	874305	1034348	22.26%	2.346%
21	19.286	2733	2737	2741	rVV	269831	355239	7.65%	0.806%
22	19.339	2742	2746	2751	rVV	199937	261333	5.62%	0.593%
23	19.404	2751	2757	2768	rVV3	173108	302186	6.50%	0.685%
24	19.651	2795	2799	2807	rVB	342593	489816	10.54%	1.111%
25	19.780	2818	2821	2826	rBV2	48862	76186	1.64%	0.173%
26	19.856	2829	2834	2839	rBV	4080596	4646679	100.00%	10.538%
27	20.492	2940	2942	2946	rVB2	74209	80806	1.74%	0.183%
28	21.127	3047	3050	3059	rVB2	368100	538512	11.59%	1.221%
29	21.421	3094	3100	3104	rBV	1723417	2456912	52.87%	5.572%
30	22.015	3198	3201	3204	rVV	201462	214762	4.62%	0.487%
31	22.050	3204	3207	3214	rVB2	219912	327598	7.05%	0.743%
32	23.050	3373	3377	3384	rBV2	425136	709908	15.28%	1.610%
33	23.791	3497	3503	3510	rVB	1099924	2093635	45.06%	4.748%
34	24.362	3595	3600	3610	rVB	620392	1215772	26.16%	2.757%
35	27.744	4167	4175	4193	rVB3	915250	3830101	82.43%	8.686%
36	28.503	4296	4304	4323	rVB5	824263	3315393	71.35%	7.519%

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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-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

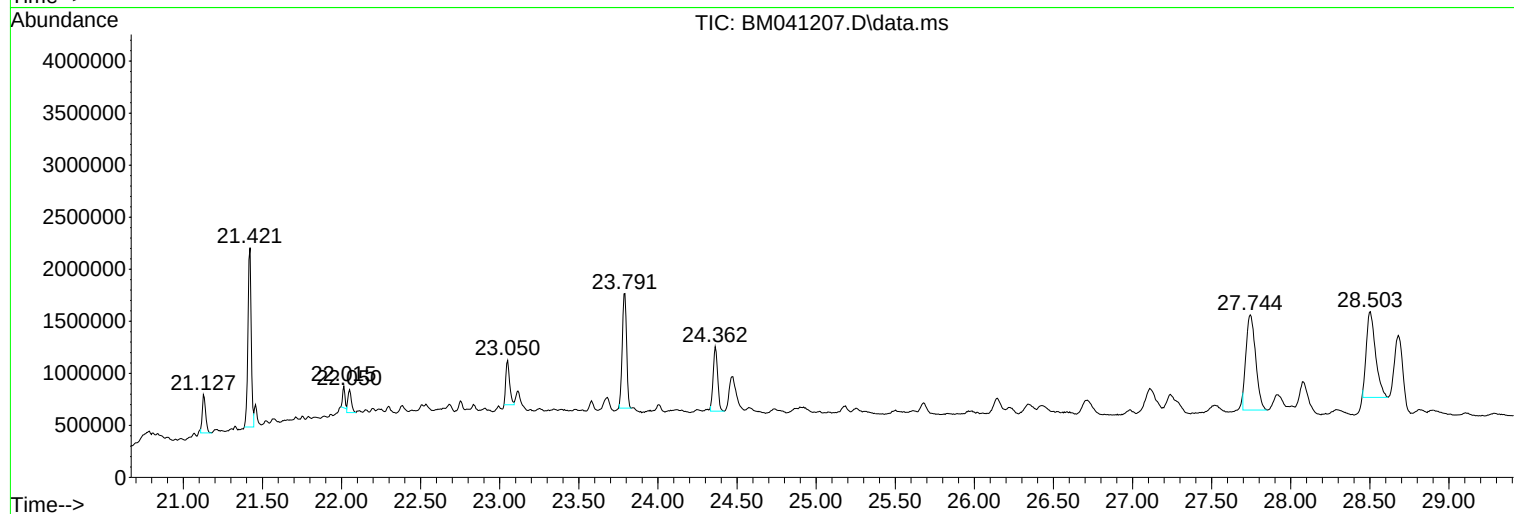
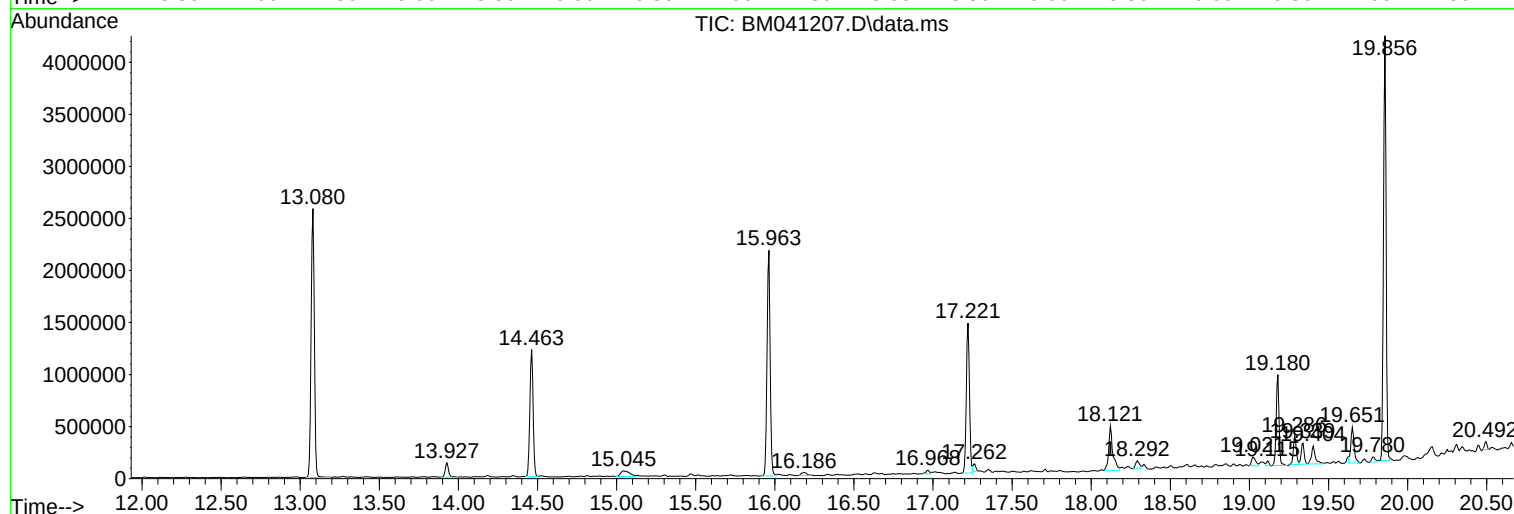
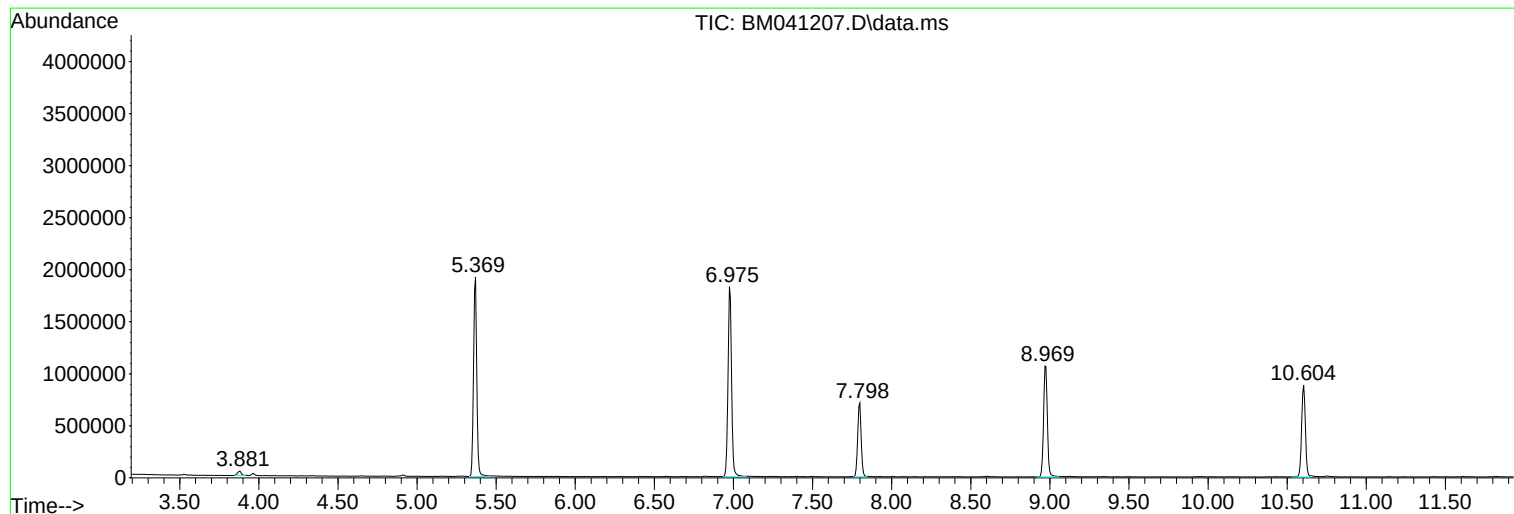
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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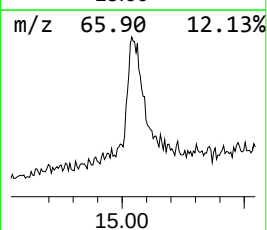
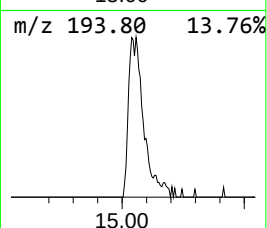
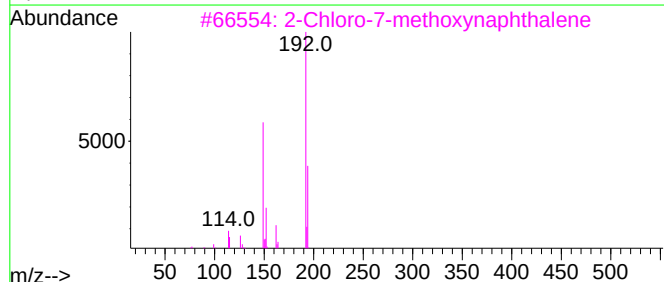
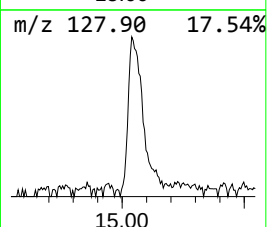
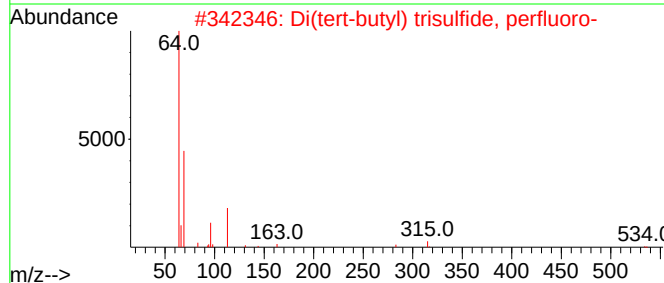
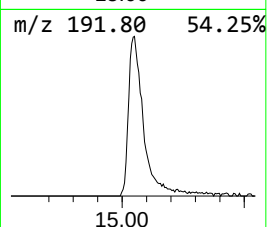
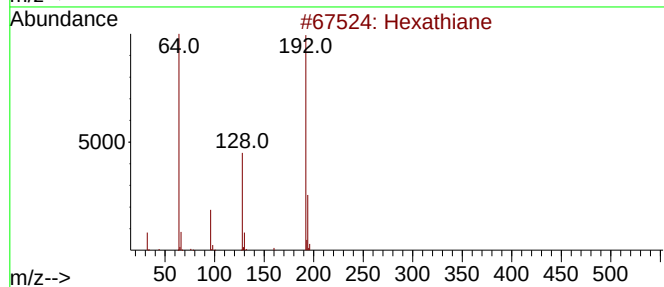
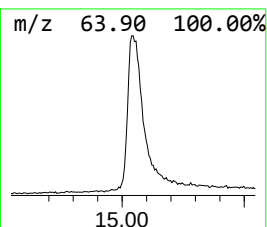
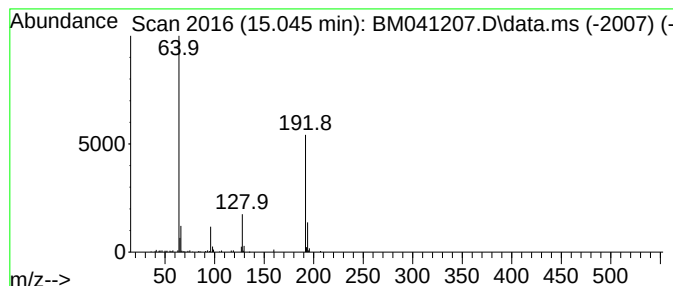
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexathiane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	2.52 ng	218155	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	91
2			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	39
3			2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	7
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	5
5			dimethyl tellurenyl	192	C2H6STe	1000374-19-6	5



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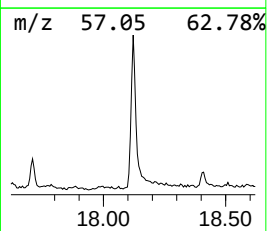
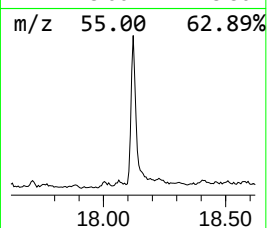
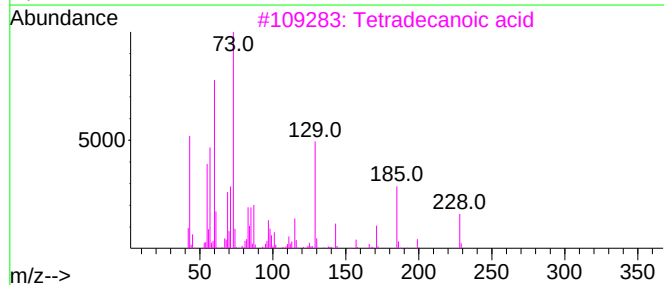
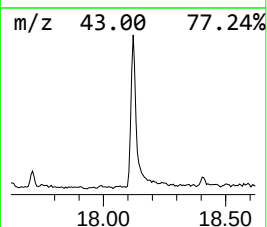
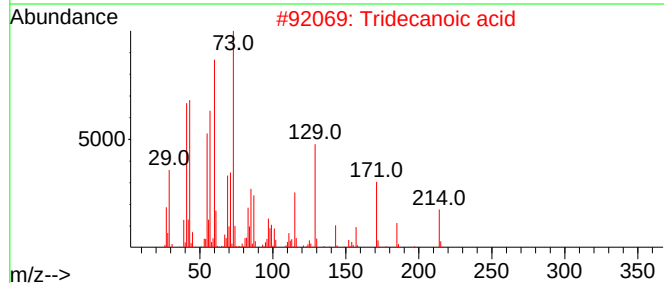
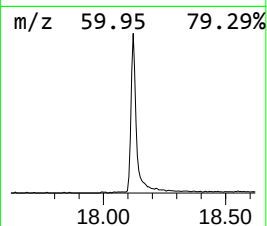
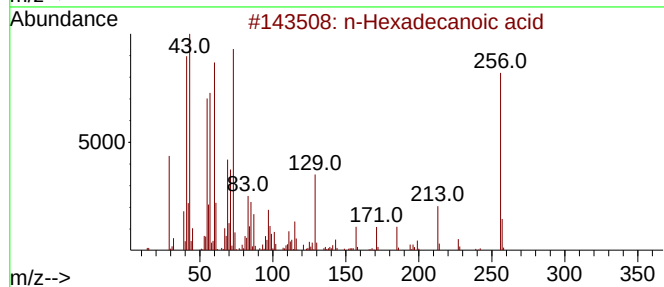
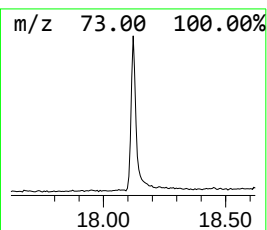
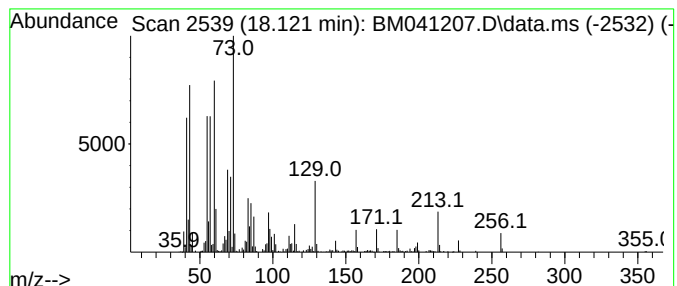
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	7.65 ng	770610	Phenanthrene-d10	17.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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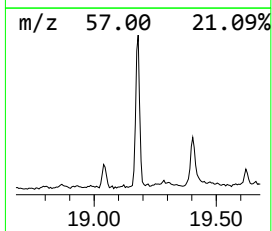
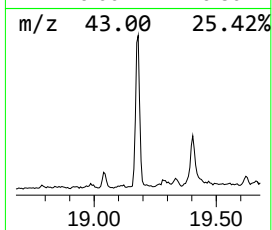
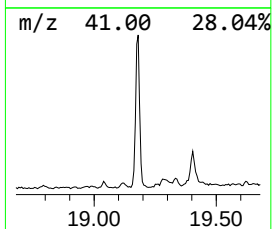
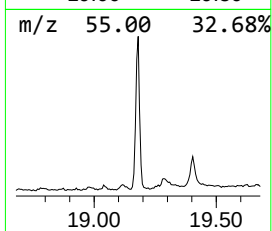
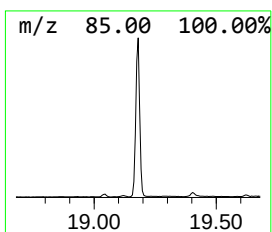
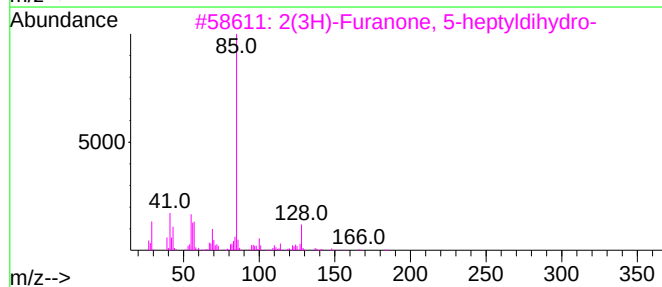
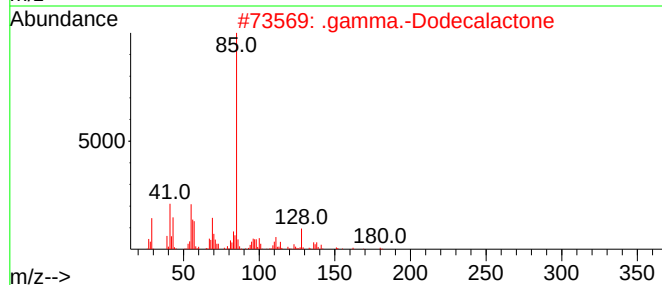
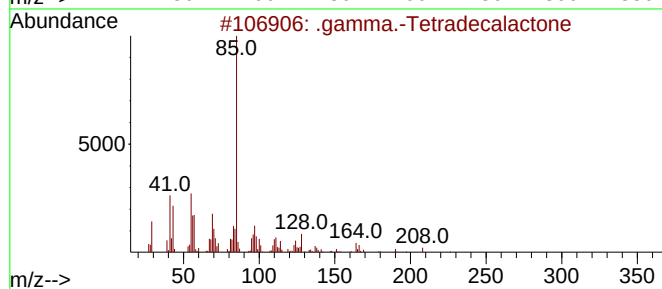
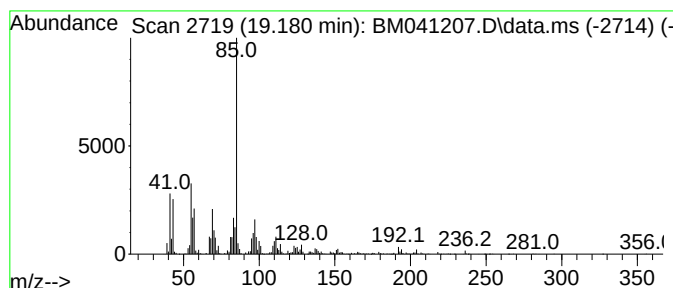
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 .gamma.-Tetradecalactone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.180	10.27 ng	1034350	Phenanthrene-d10	17.221	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Tetradecalactone	226	C14H26O2	002721-23-5	78
2	.gamma.-Dodecalactone	198	C12H22O2	002305-05-7	72
3	2(3H)-Furanone, 5-heptyldihydro-	184	C11H20O2	000104-67-6	59
4	1-Bromo-7-(tetrahydro-2-pyranylo...	278	C12H23BrO2	010160-25-5	59
5	Pentanoic acid, 4-hexadecyl ester	326	C21H42O2	1000282-86-4	59



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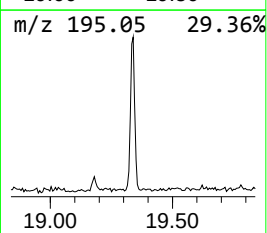
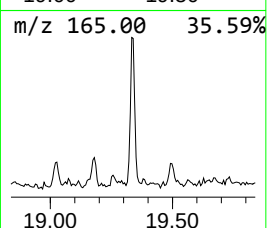
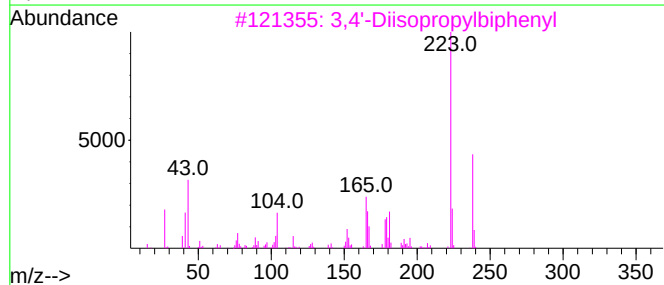
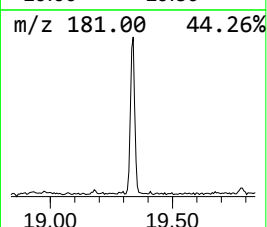
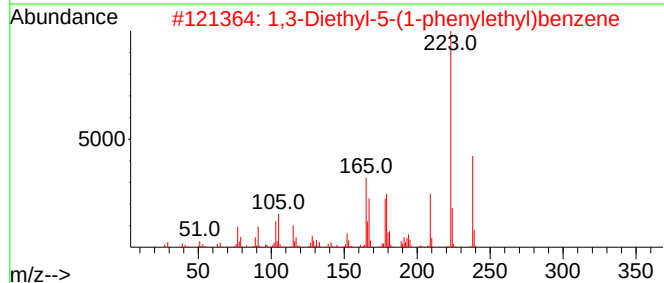
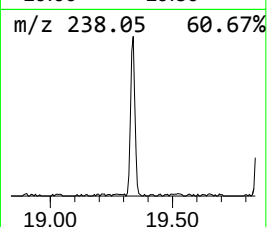
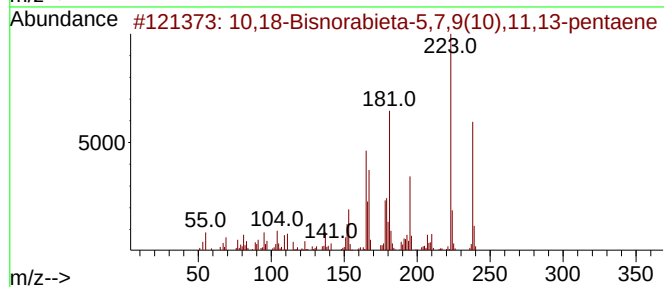
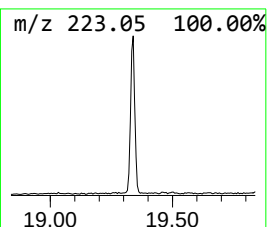
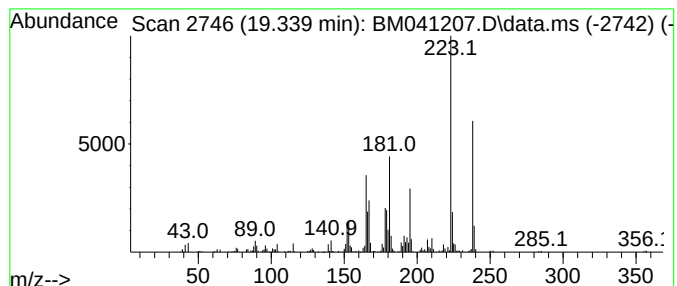
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.339	2.13 ng	261333	Chrysene-d12	21.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	98
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	89
3	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	76
4	Anthracene, 1,4-dimethoxy-	238	C16H14O2	013076-29-4	55
5	Anthracene, 9,10-dimethoxy-	238	C16H14O2	002395-97-3	50



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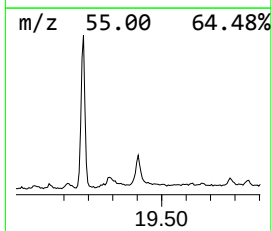
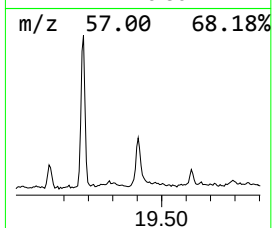
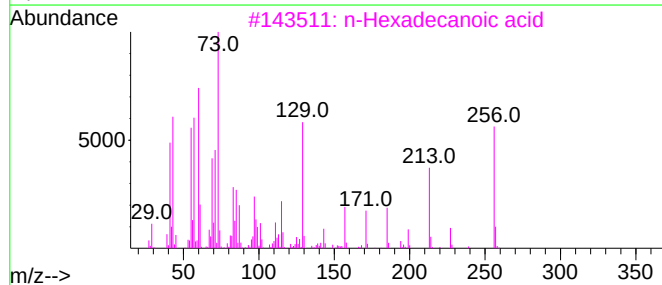
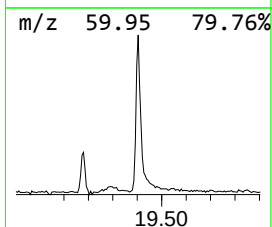
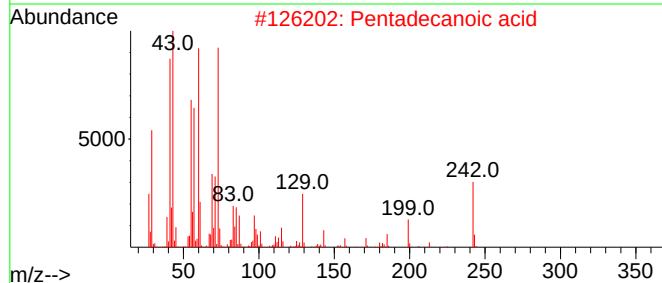
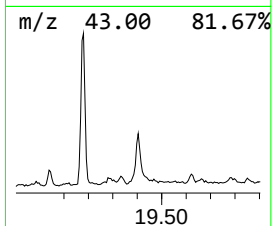
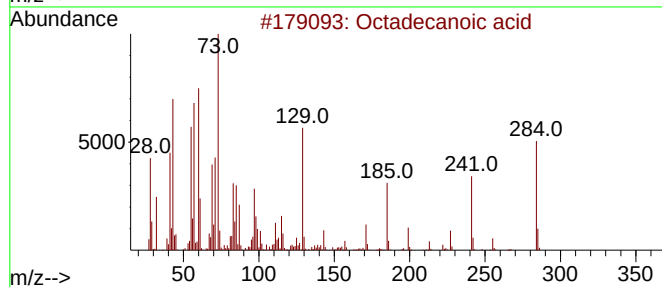
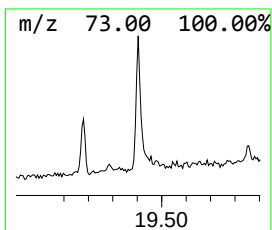
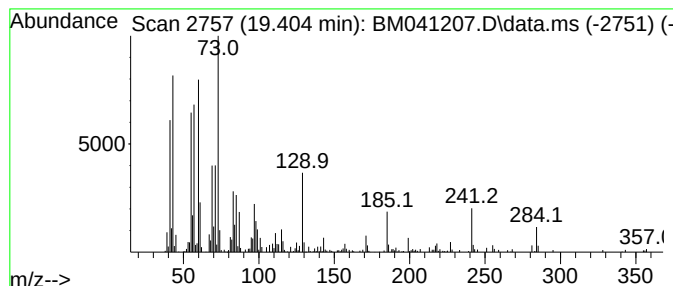
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	2.46 ng	302186	Chrysene-d12	21.421

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	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041207.D
Acq On : 01 Aug 2023 03:18
Operator : MA/JU
Sample : 03741-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P6B

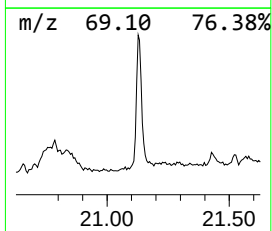
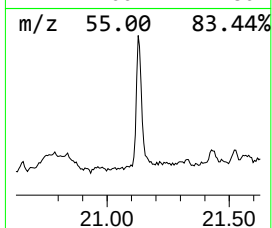
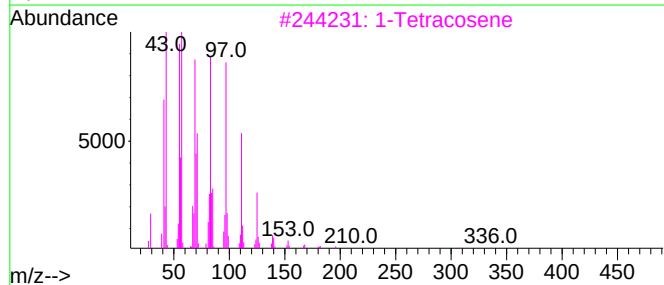
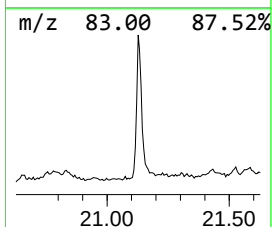
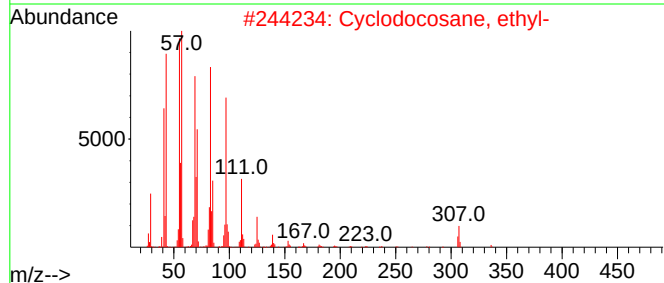
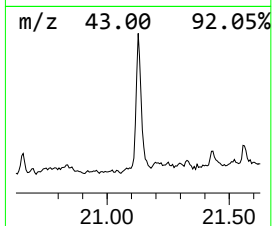
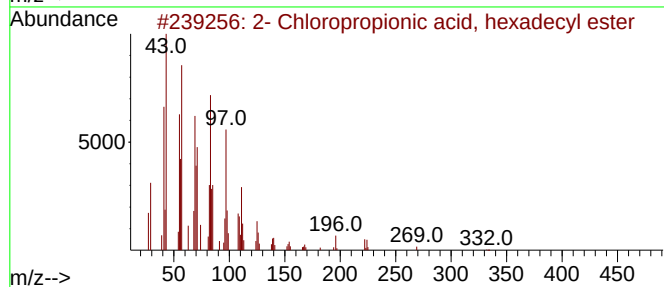
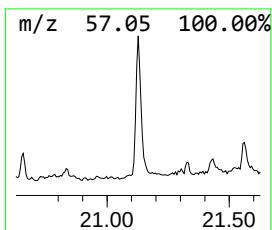
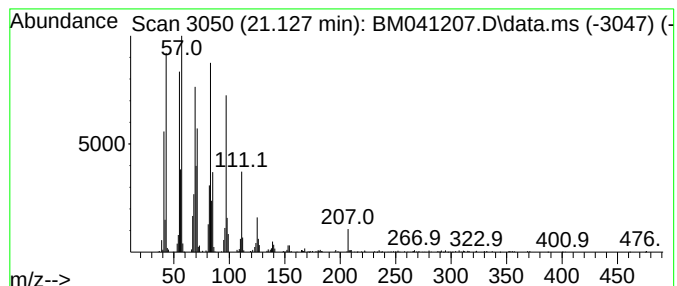
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2- Chloropropionic acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.38 ng	538512	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93
2			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
3			1-Tetracosene	336	C24H48	010192-32-2	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041207.D
Acq On : 01 Aug 2023 03:18
Operator : MA/JU
Sample : 03741-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

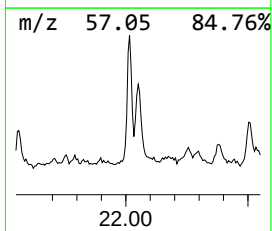
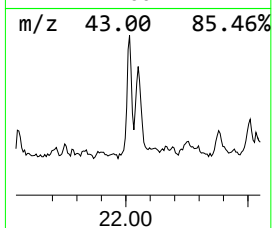
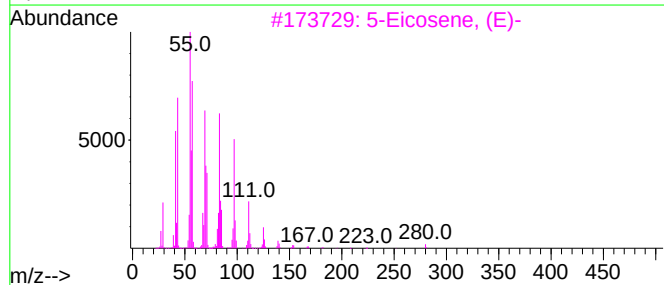
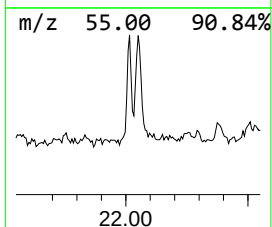
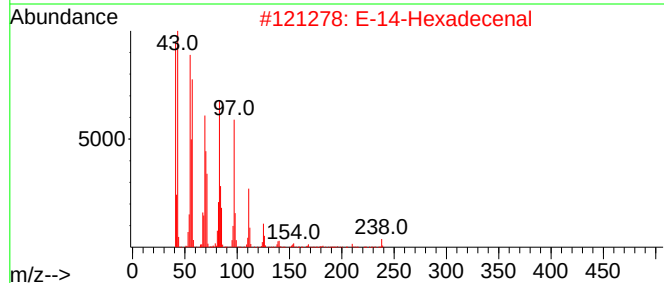
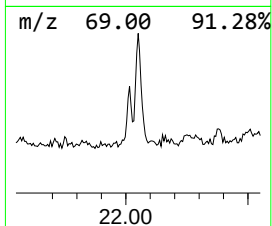
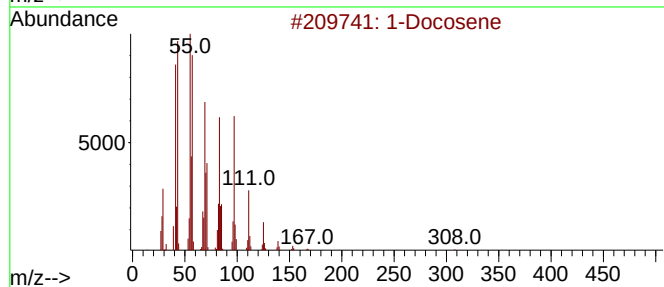
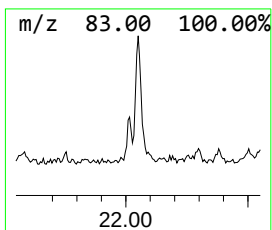
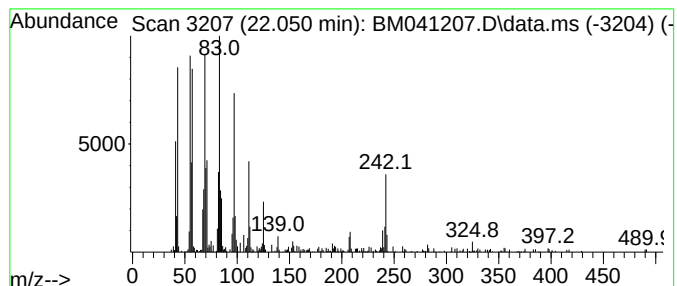
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.050	2.67 ng	327598	Chrysene-d12	21.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	96
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	95
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
4	1-Tetracosene	336	C24H48	010192-32-2	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041207.D
Acq On : 01 Aug 2023 03:18
Operator : MA/JU
Sample : 03741-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

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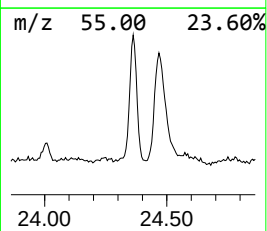
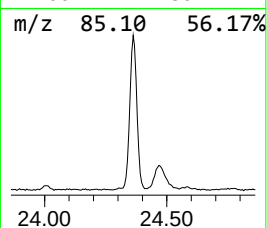
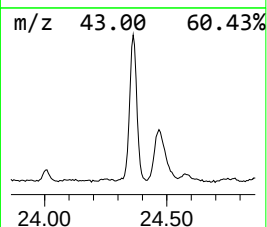
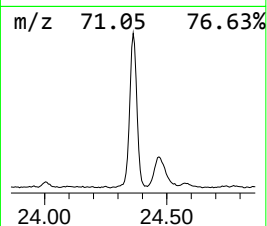
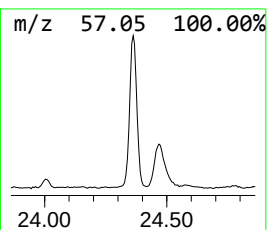
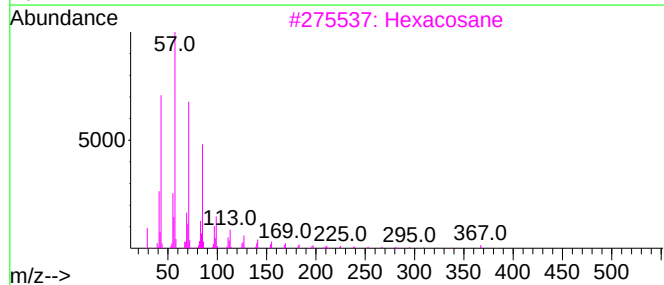
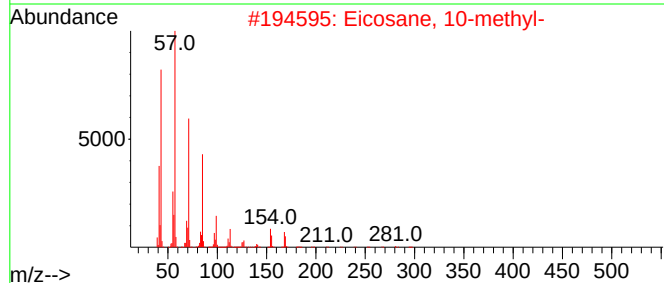
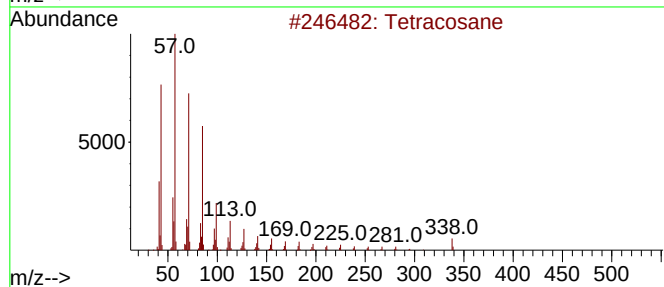
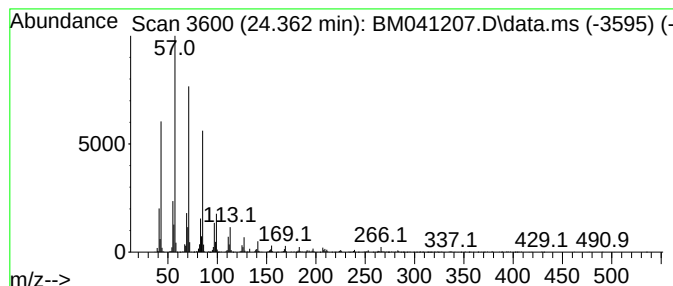
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.362	11.61 ng	1215770	Perylene-d12	23.791

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	94
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5			2-Methylheptacosane	394	C28H58	001561-00-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041207.D
Acq On : 01 Aug 2023 03:18
Operator : MA/JU
Sample : 03741-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P6B

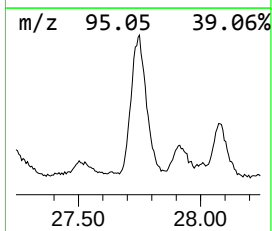
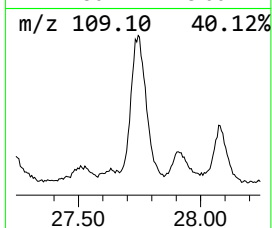
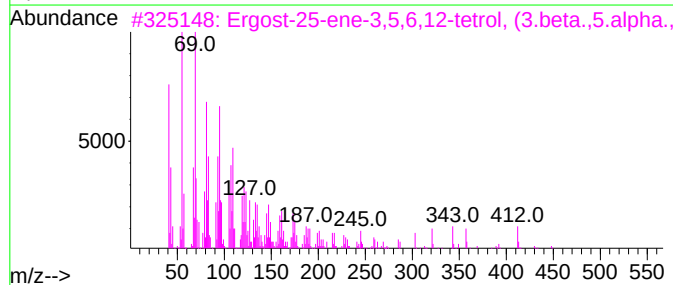
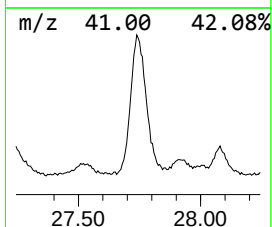
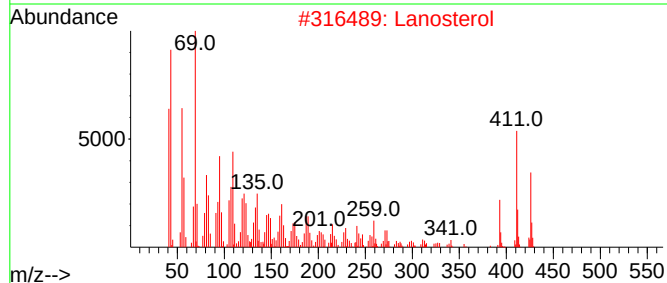
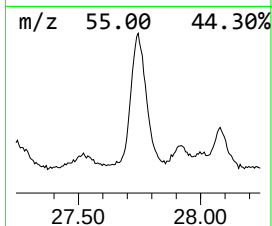
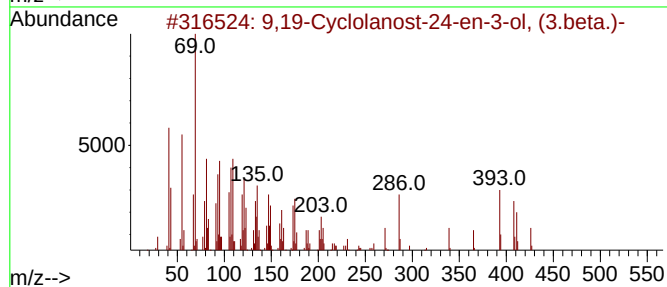
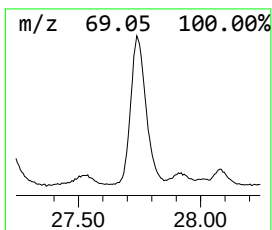
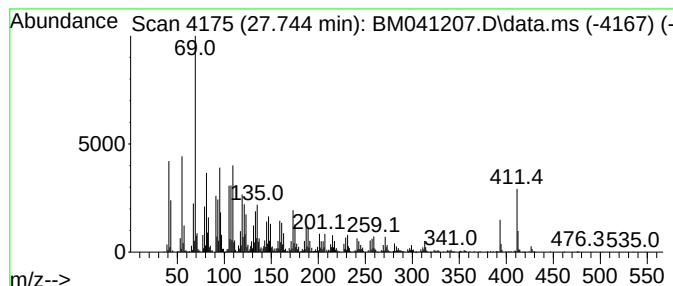
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9,19-Cyclolanost-24-en-3-ol... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.744	36.59 ng	3830100	Perylene-d12	23.791

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, (3...	426	C30H50O	000469-38-5	91		
2	Lanosterol	426	C30H50O	000079-63-0	12		
3	Ergost-25-ene-3,5,6,12-tetrol, (...	448	C28H48O4	056052-97-2	12		
4	Cycloprop[7,8]ergost-22-en-3-ol,...	412	C29H48O	053866-87-8	9		
5	1,1,1,2,5,5,6,6,6-Nonafluoro-3-(...	500	C10F20	1000461-21-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041207.D
Acq On : 01 Aug 2023 03:18
Operator : MA/JU
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-P6B

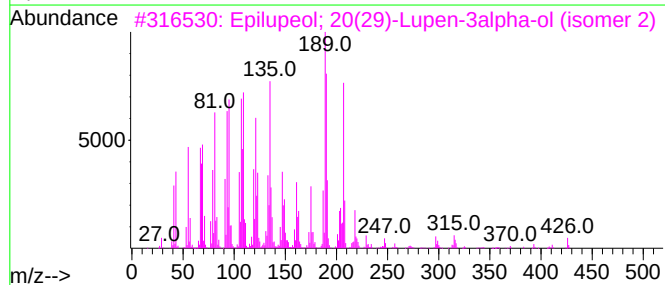
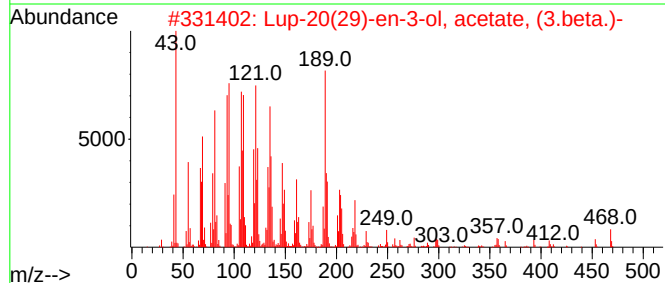
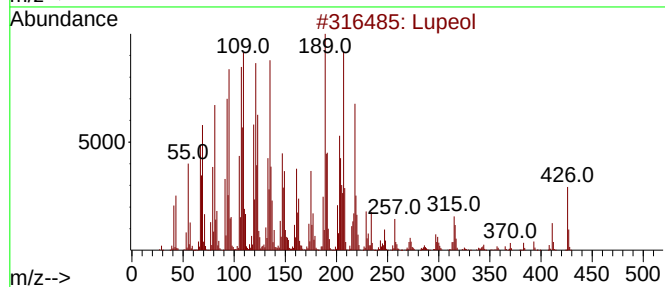
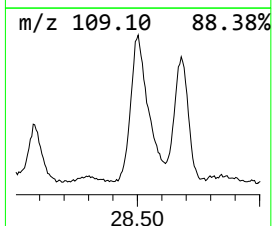
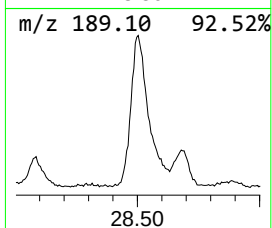
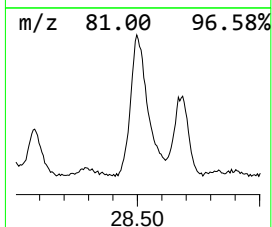
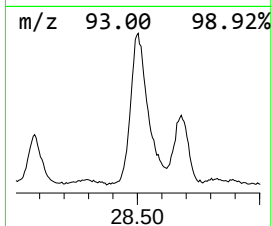
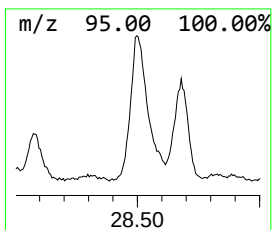
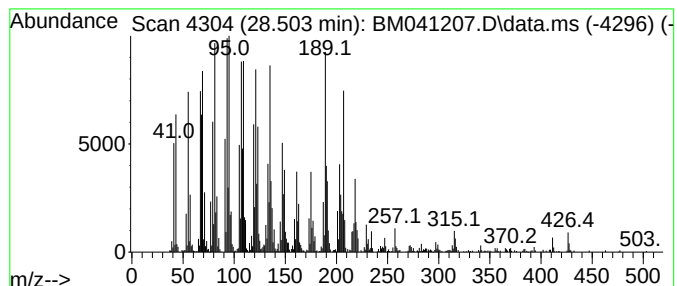
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Lupeol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.503	31.67 ng	3315390	Perylene-d12	23.791

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	99
2			Lup-20(29)-en-3-ol, acetate, (3....	468	C32H52O2	001617-68-1	91
3			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	86
4			Thunbergol	290	C20H34O	025269-17-4	83
5			Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041207.D
Acq On : 01 Aug 2023 03:18
Operator : MA/JU
Sample : 03741-13
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P6B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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 ...	18.121	7.7	ng	770610	4	17.221	2015050	20.0
.gamma.-Tetradec...	19.180	10.3	ng	1034350	4	17.221	2015050	20.0
10,18-Bisnorabi...	19.339	2.1	ng	261333	5	21.421	2456910	20.0
Octadecanoic acid	19.404	2.5	ng	302186	5	21.421	2456910	20.0
2-Chloropropio...	21.127	4.4	ng	538512	5	21.421	2456910	20.0
1-Docosene	22.050	2.7	ng	327598	5	21.421	2456910	20.0
Tetracosane	24.362	11.6	ng	1215770	6	23.791	2093640	20.0
9,19-Cyclolanos...	27.744	36.6	ng	3830100	6	23.791	2093640	20.0
Lupeol	28.503	31.7	ng	3315390	6	23.791	2093640	20.0