

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
 Data File : BM041230.D
 Acq On : 01 Aug 2023 18:23
 Operator : MA/JU
 Sample : 03715-08
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 T842-FH-04-BW

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: BM041230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.375	365	372	383	rBV	1880056	2709811	37.24%	4.712%
2	6.987	635	646	661	rBV	1827958	2946512	40.49%	5.124%
3	7.798	774	784	792	rBV	562190	867246	11.92%	1.508%
4	8.975	975	984	1001	rBV	1110094	1843725	25.34%	3.206%
5	10.604	1253	1261	1267	rBV	672586	1134714	15.59%	1.973%
6	13.080	1675	1682	1693	rBV	2994782	4414489	60.67%	7.677%
7	13.927	1818	1826	1834	rBV	162087	238014	3.27%	0.414%
8	14.116	1852	1858	1871	rBV	414645	743767	10.22%	1.293%
9	14.469	1911	1918	1928	rBV	981183	1441126	19.80%	2.506%
10	14.892	1984	1990	1998	rBV3	56984	88087	1.21%	0.153%
11	15.839	2141	2151	2163	rBV	2091546	2856177	39.25%	4.967%
12	15.968	2167	2173	2179	rBV	2866565	3904289	53.65%	6.790%
13	17.227	2381	2387	2393	rBV	1248854	1755724	24.13%	3.053%
14	18.133	2535	2541	2566	rBV	2878604	4277461	58.78%	7.439%
15	19.292	2735	2738	2750	rVB3	120453	250666	3.44%	0.436%
16	19.409	2754	2758	2778	rVV	2508258	3603070	49.52%	6.266%
17	19.739	2809	2814	2827	rBV	466468	938518	12.90%	1.632%
18	19.862	2830	2835	2849	rVB	6433357	7276700	100.00%	12.654%
19	21.133	3047	3051	3057	rBV2	325552	437525	6.01%	0.761%
20	21.427	3097	3101	3108	rBV	1502908	1836505	25.24%	3.194%
21	23.803	3499	3505	3512	rVB	1012983	1937437	26.63%	3.369%
22	24.233	3572	3578	3588	rVB	2479977	4992708	68.61%	8.682%
23	28.215	4244	4255	4272	rVB	1930378	7008940	96.32%	12.189%

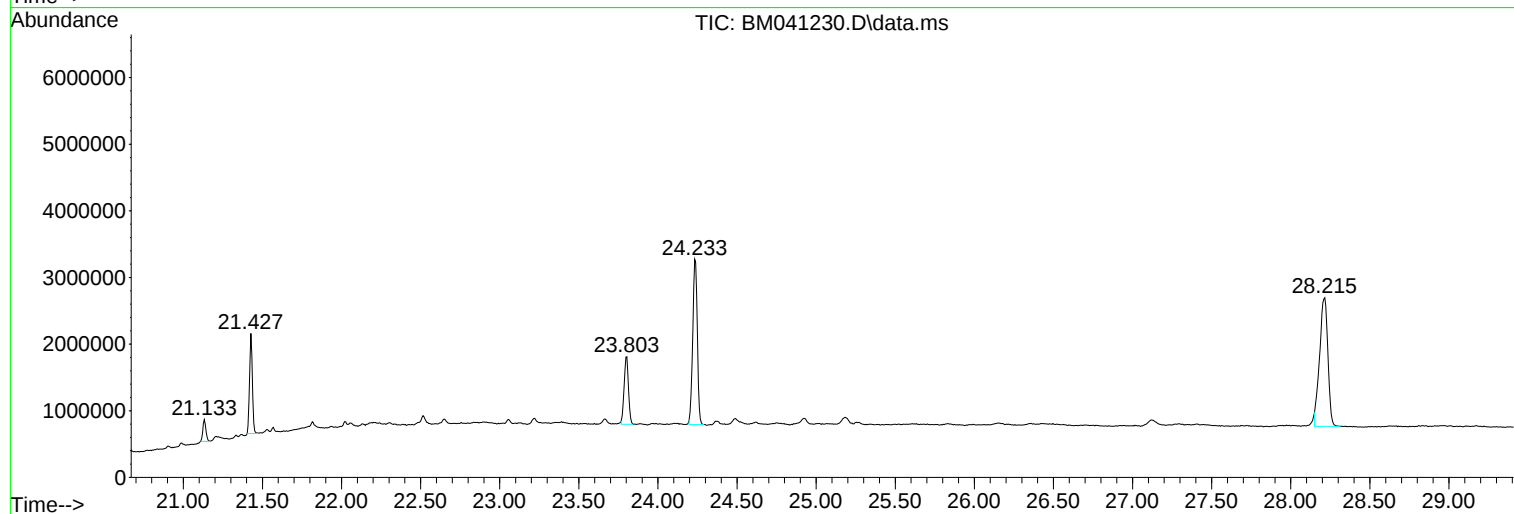
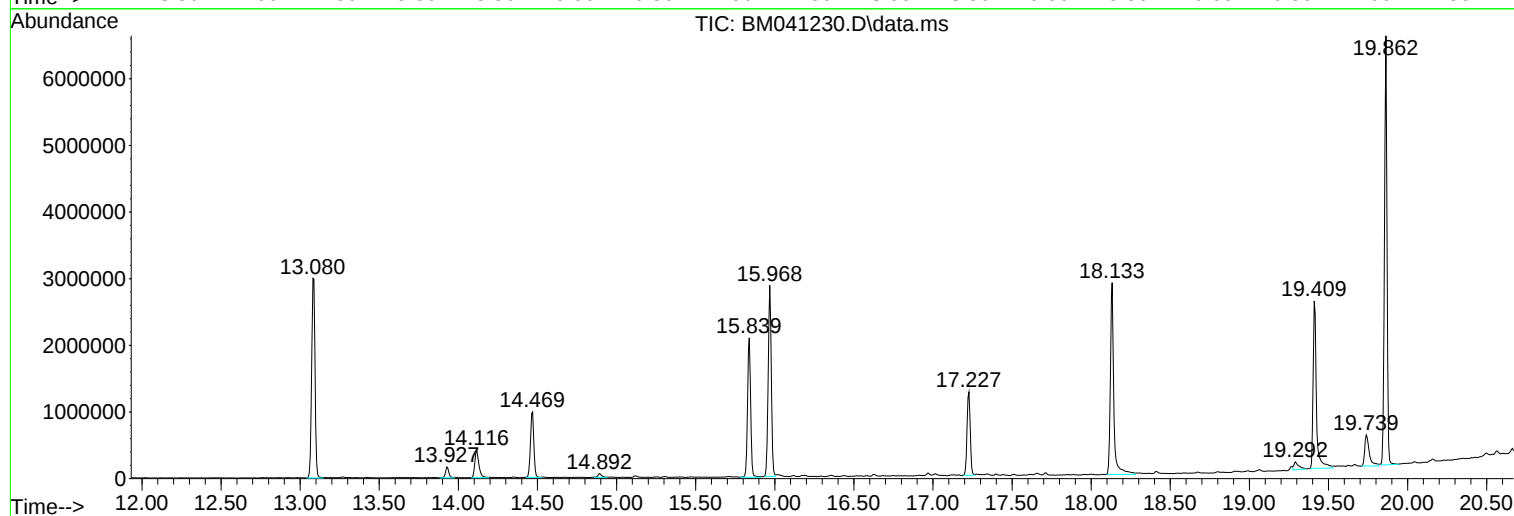
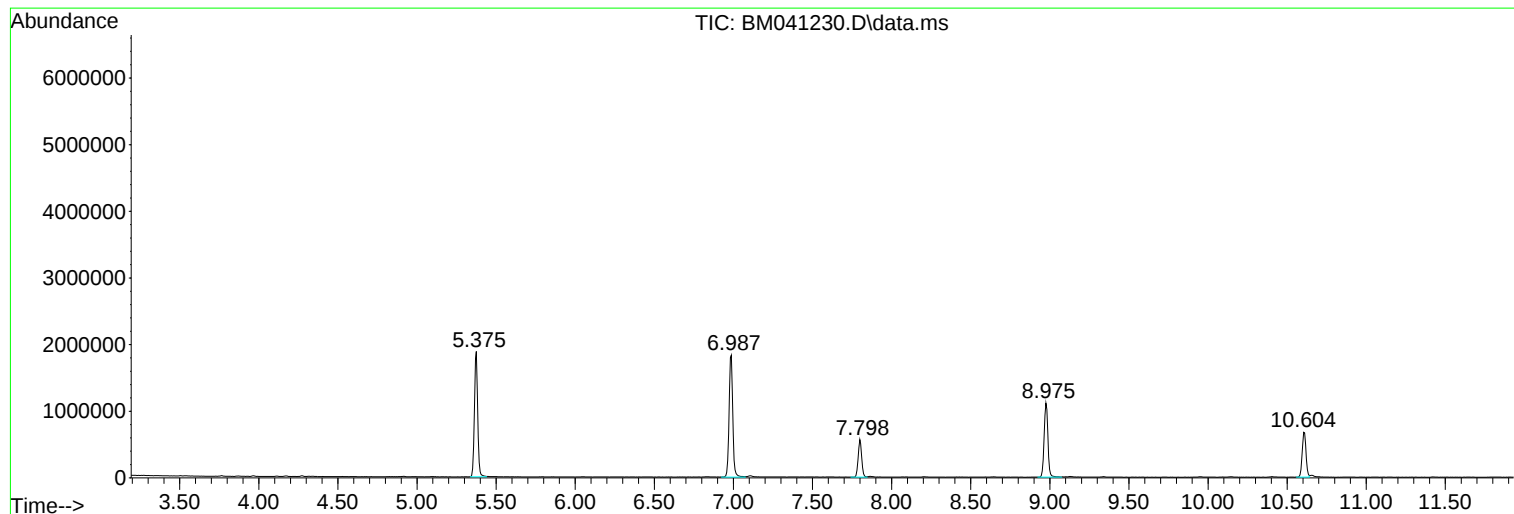
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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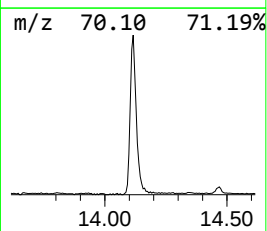
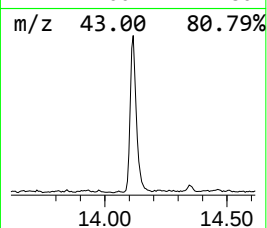
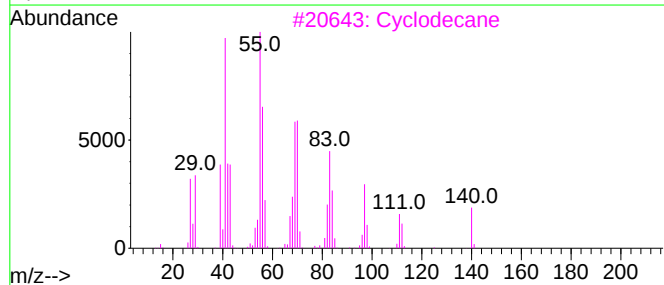
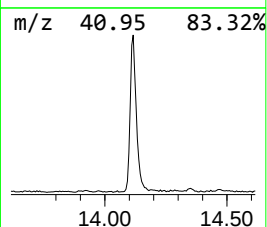
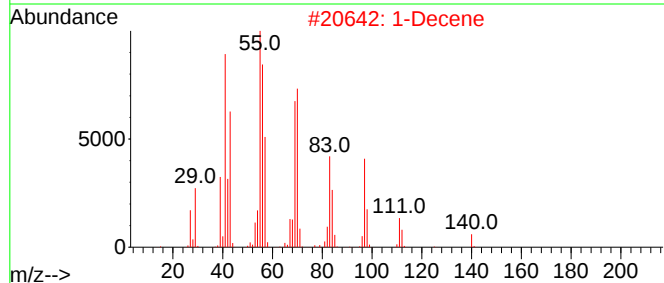
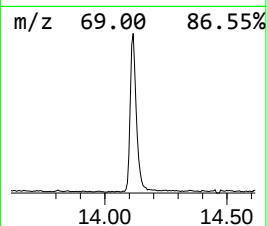
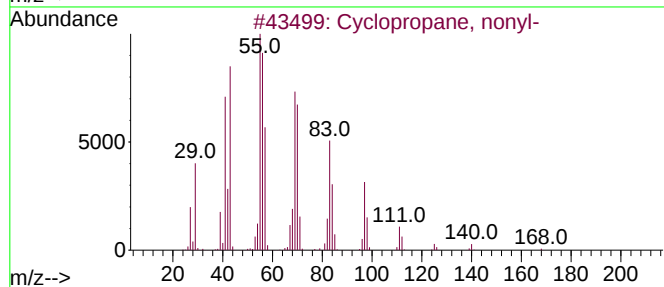
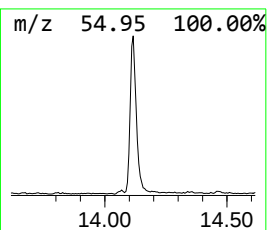
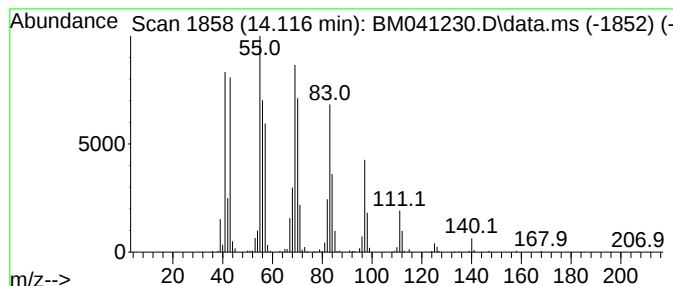
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopropane, nonyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.116	10.32 ng	743767	Acenaphthene-d10	14.469

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, nonyl-	168	C12H24	074663-85-7	95
2		1-Decene	140	C10H20	000872-05-9	95
3		Cyclodecane	140	C10H20	000293-96-9	94
4		1-Undecanol	172	C11H24O	000112-42-5	91
5		Cyclododecane	168	C12H24	000294-62-2	91



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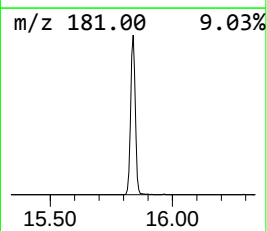
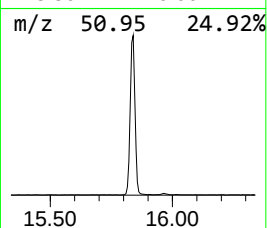
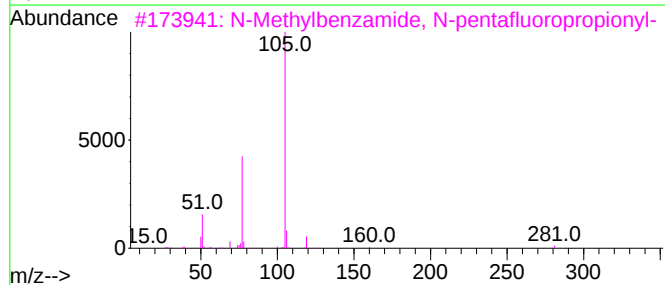
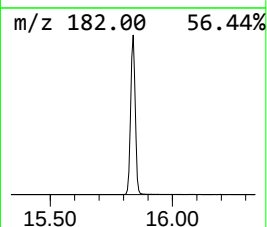
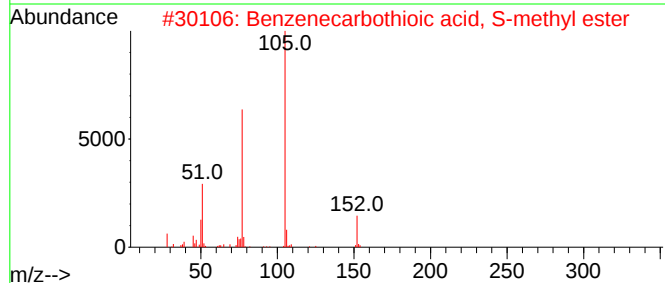
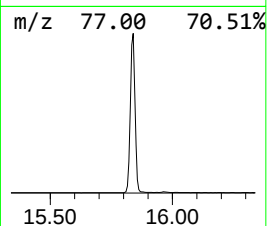
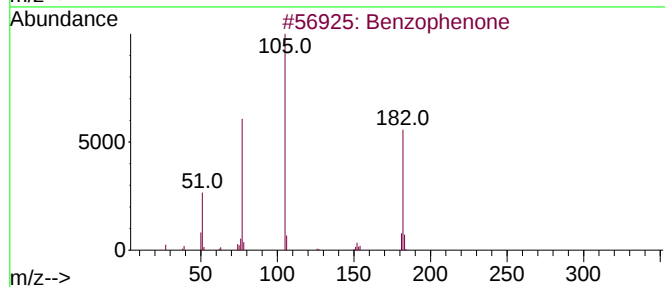
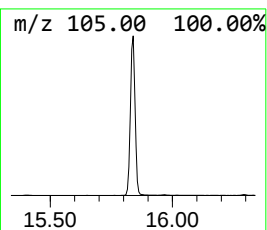
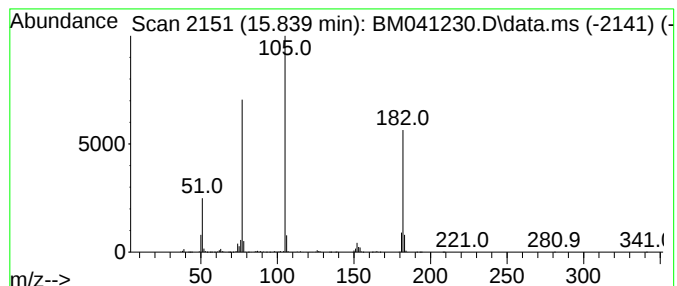
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	39.64 ng	2856180	Acenaphthene-d10	14.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47



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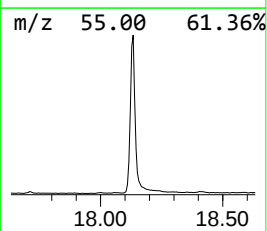
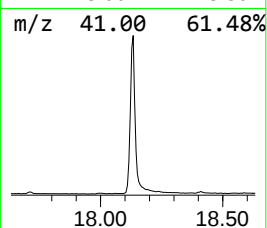
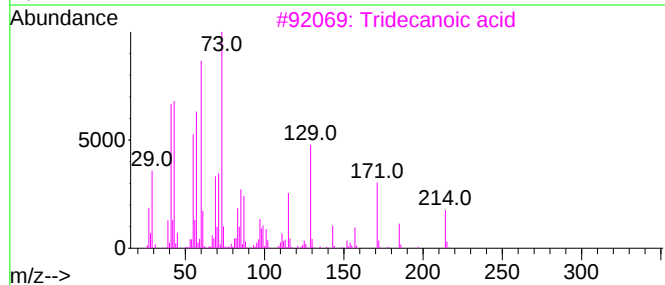
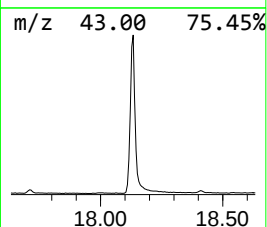
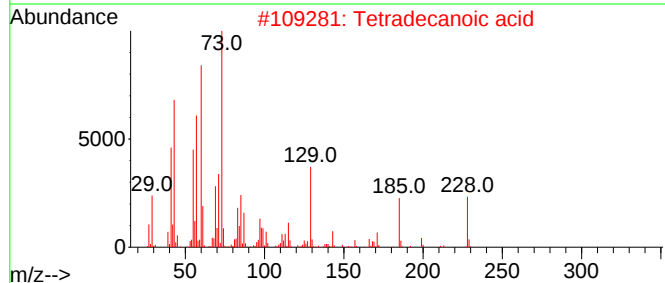
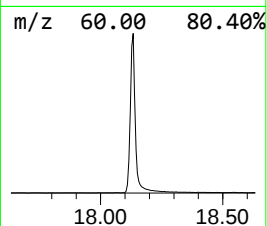
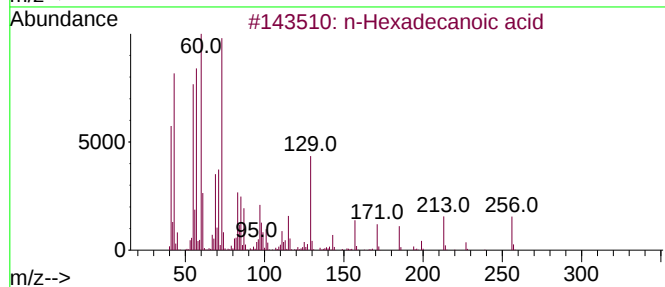
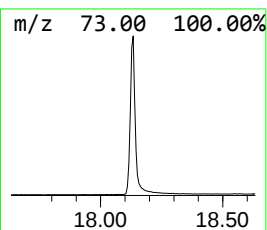
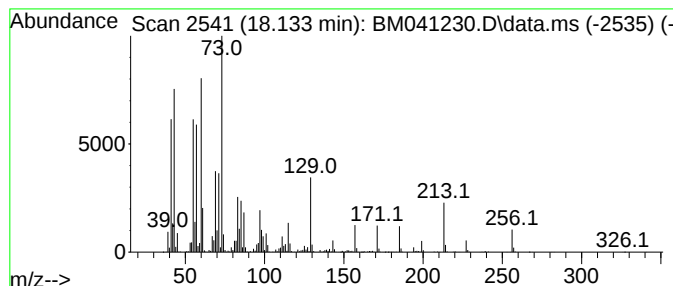
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.133	48.73 ng	4277460	Phenanthrene-d10	17.227

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			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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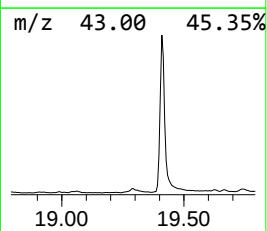
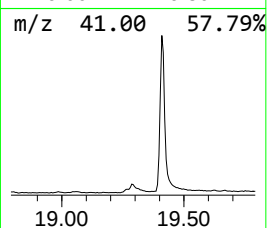
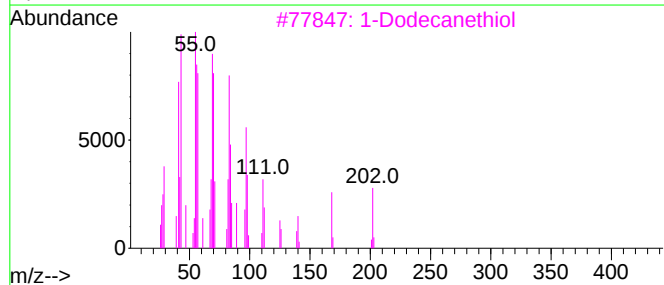
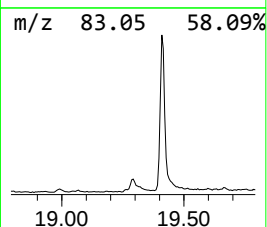
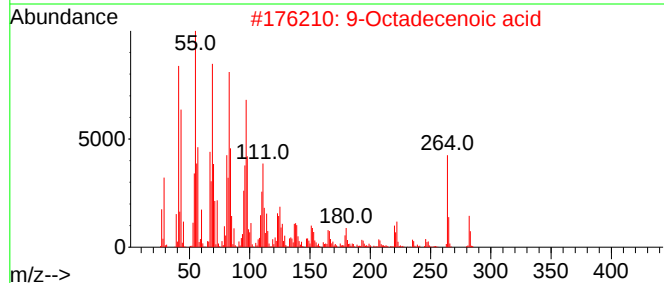
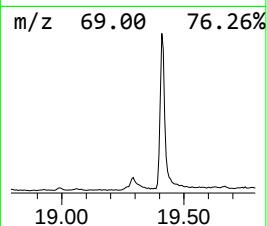
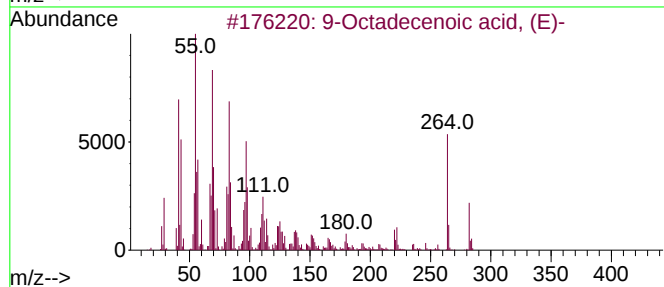
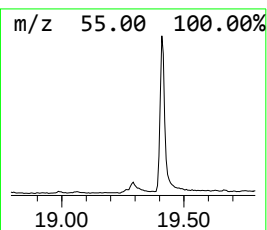
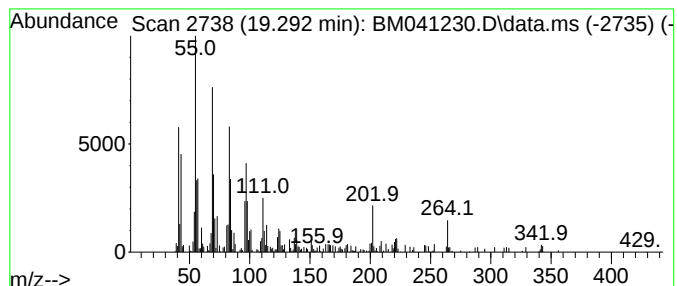
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.292	2.86 ng	250666	Phenanthrene-d10	17.227

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
2		9-Octadecenoic acid	282	C18H34O2	002027-47-6	87
3		1-Dodecanethiol	202	C12H26S	000112-55-0	87
4		Oleic Acid	282	C18H34O2	000112-80-1	86
5		14-Pentadecenoic acid	240	C15H28O2	017351-34-7	80



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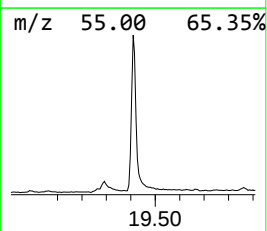
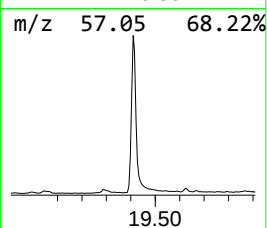
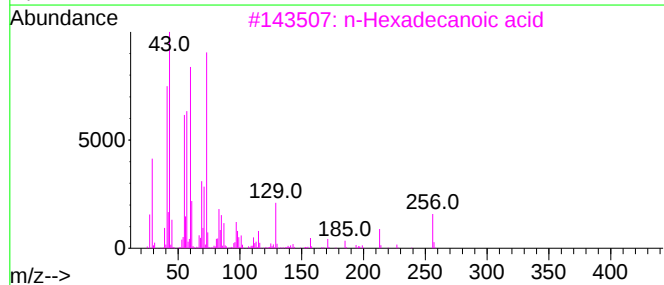
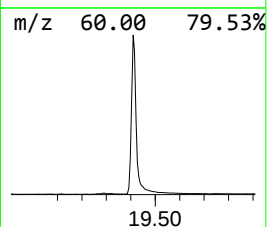
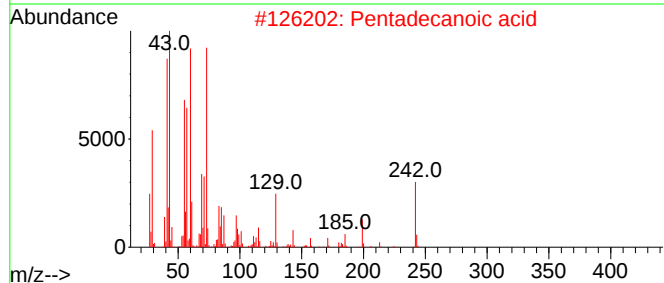
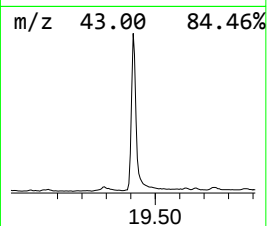
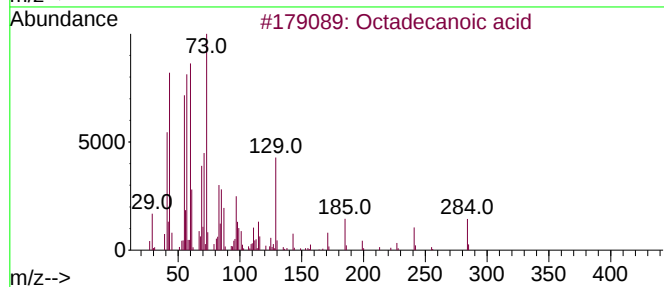
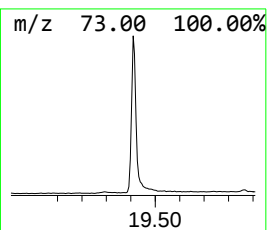
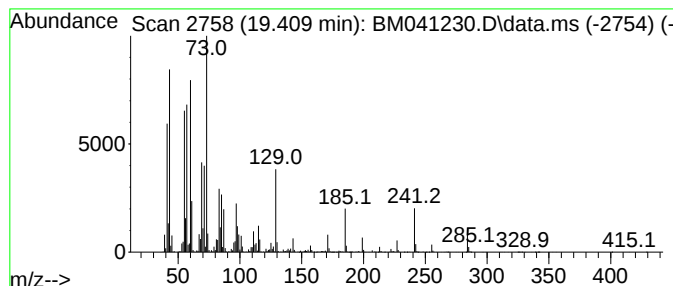
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.409	39.24 ng	3603070	Chrysene-d12	21.427

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	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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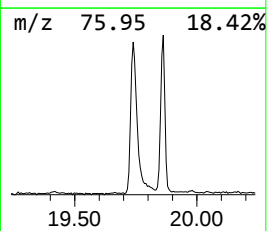
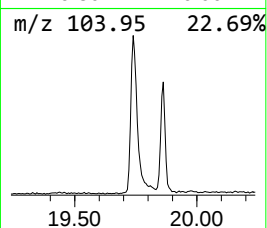
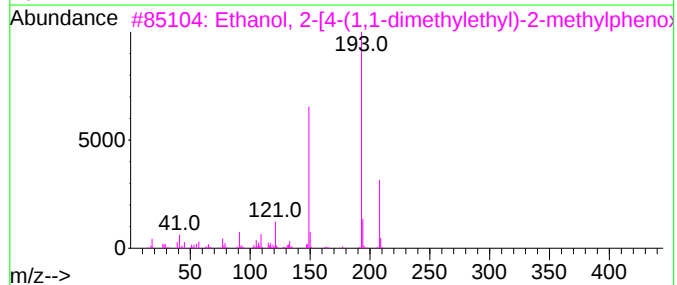
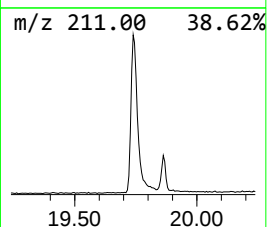
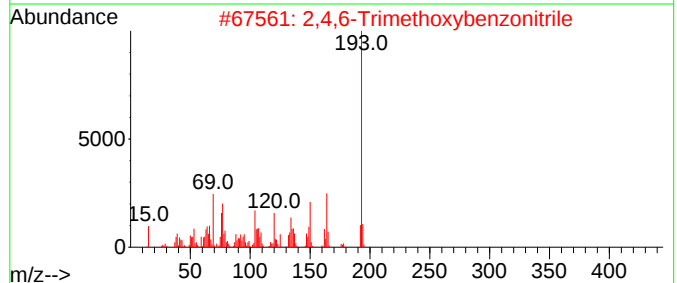
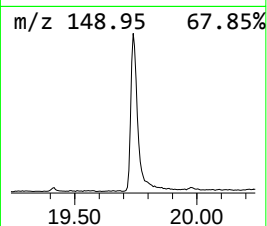
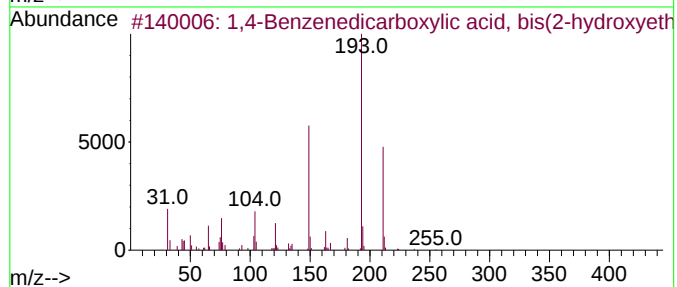
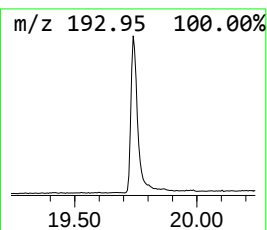
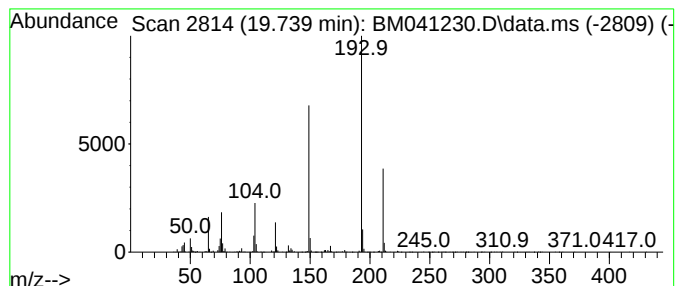
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ClientSampleId :
T842-FH-04-BW

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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 1,4-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
19.739	10.22 ng	938518	Chrysene-d12			21.427
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...		254	C12H14O6	000959-26-2	83
2	2,4,6-Trimethoxybenzonitrile		193	C10H11NO3	002571-54-2	43
3	Ethanol, 2-[4-(1,1-dimethylethyl...		208	C13H20O2	054934-87-1	38
4	2-(Propoxycarbonyl)benzoic acid		208	C11H12O4	1000373-63-1	22
5	2-((But-3-enyloxy)carbonyl)benzo...		220	C12H12O4	113793-34-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041230.D
Acq On : 01 Aug 2023 18:23
Operator : MA/JU
Sample : 03715-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-BW

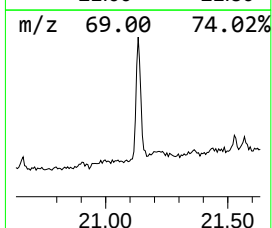
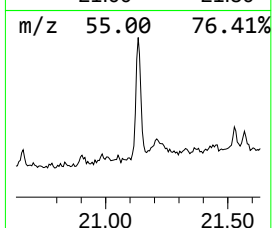
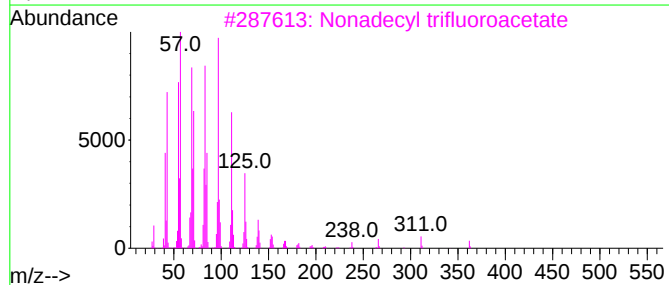
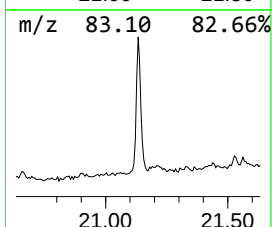
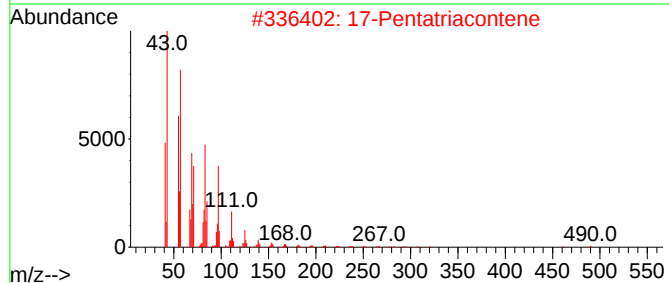
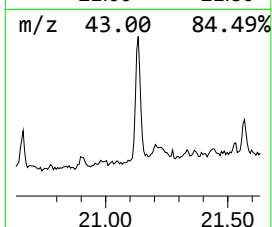
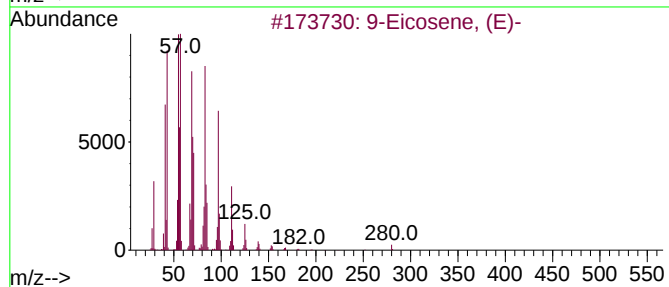
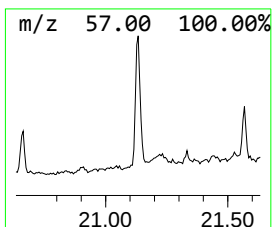
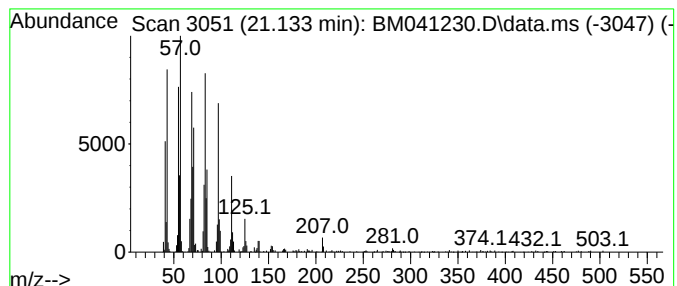
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	4.76 ng	437525	Chrysene-d12	21.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Eicosene, (E)-	280	C20H40	074685-29-3	93
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5		Pentacos-1-ene	350	C25H50	016980-85-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041230.D
Acq On : 01 Aug 2023 18:23
Operator : MA/JU
Sample : 03715-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-BW

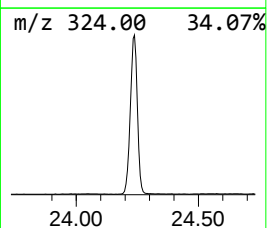
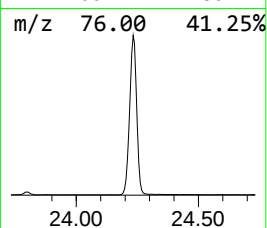
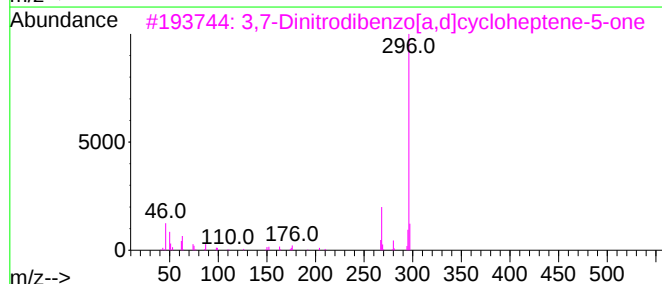
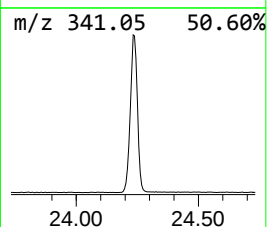
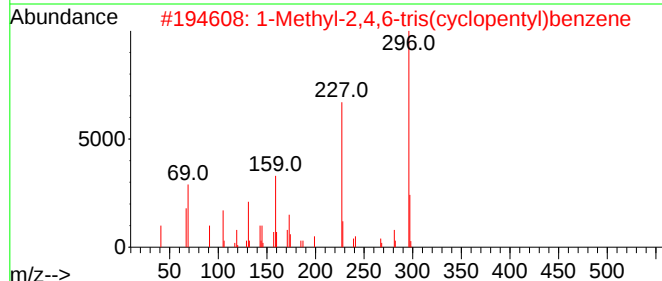
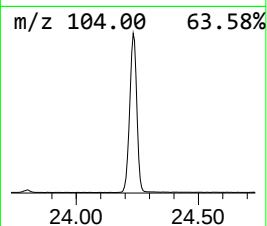
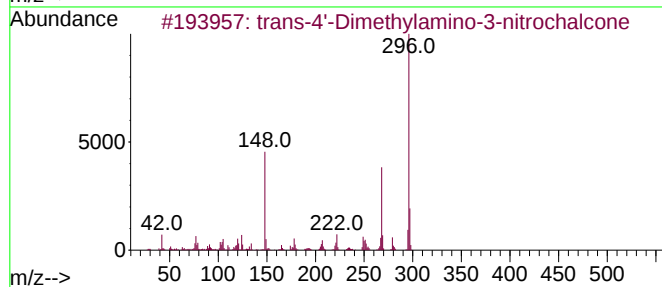
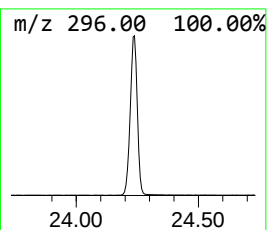
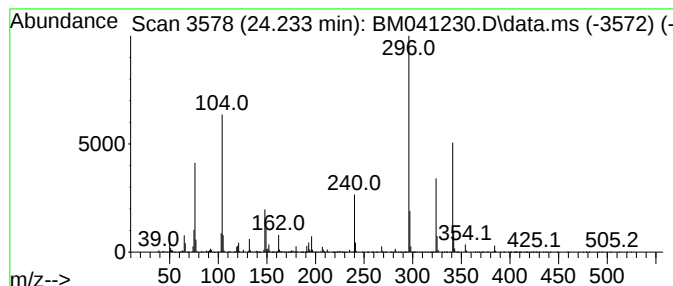
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown24.233 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.233	51.54 ng	4992710	Perylene-d12	23.803

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4'-Dimethylamino-3-nitroch...	296	C17H16N2O3	1000234-56-7	16
2			1-Methyl-2,4,6-tris(cyclopentyl)...	296	C22H32	100325-74-4	14
3			3,7-Dinitrodibenzo[a,d]cyclohept...	296	C15H8N2O5	062417-95-2	14
4			4-[4-(4-Methoxyphenyl)-5-methyl-...	296	C17H16N2O3	394237-61-7	12
5			2-Thiazolamine, 4-(4-methoxyphen...	296	C17H16N2O5	1010319-57-2	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041230.D
Acq On : 01 Aug 2023 18:23
Operator : MA/JU
Sample : 03715-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-BW

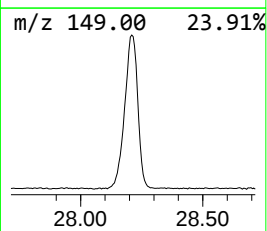
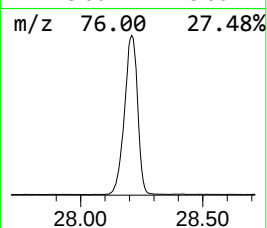
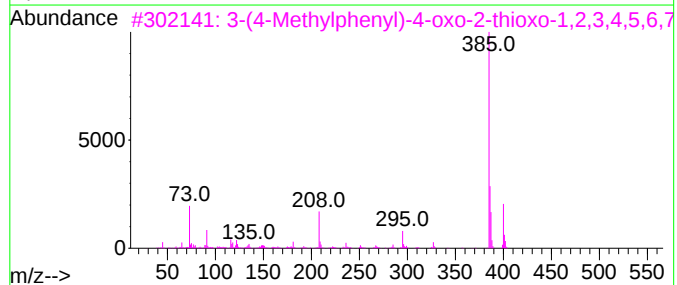
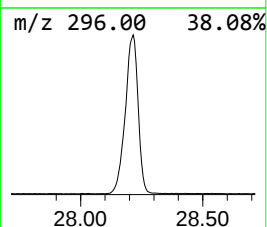
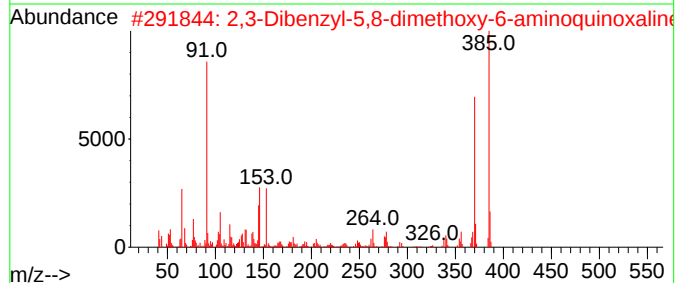
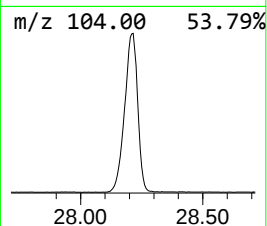
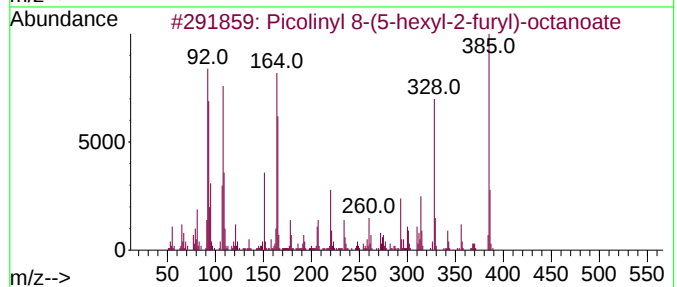
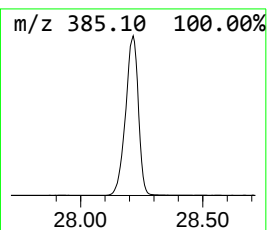
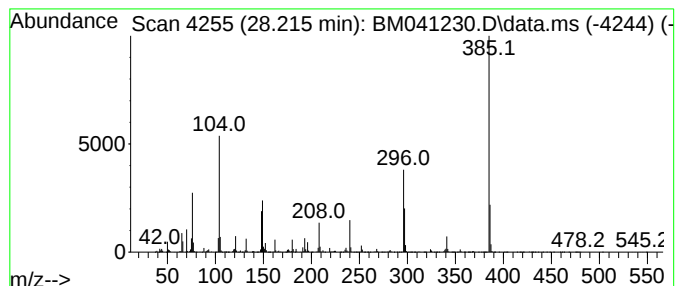
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown28.215 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.215	72.35 ng	7008940	Perylene-d12	23.803

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picolinyl 8-(5-hexyl-2-furyl)-oc...	385	C24H35NO3	1000335-93-0	38
2			2,3-Dibenzyl-5,8-dimethoxy-6-ami...	385	C24H23N3O2	056393-28-3	16
3			3-(4-Methylphenyl)-4-oxo-2-thiox...	400	C20H24N2OS2Si	1000512-11-8	12
4			3-Hydroxy-6,3',4'-trimethoxyflav...	400	C21H24O6Si	1000448-94-7	12
5			3-Hydroxy-7,2',3'-trimethoxyflav...	400	C21H24O6Si	1000448-94-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041230.D
Acq On : 01 Aug 2023 18:23
Operator : MA/JU
Sample : 03715-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-BW

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
Cyclopropane, n...	14.116	10.3	ng	743767	3	14.469	1441130	20.0
Benzophenone	15.839	39.6	ng	2856180	3	14.469	1441130	20.0
n-Hexadecanoic ...	18.133	48.7	ng	4277460	4	17.227	1755720	20.0
9-Octadecenoic ...	19.292	2.9	ng	250666	4	17.227	1755720	20.0
Octadecanoic acid	19.409	39.2	ng	3603070	5	21.427	1836510	20.0
1,4-Benzenedica...	19.739	10.2	ng	938518	5	21.427	1836510	20.0
9-Eicosene, (E)-	21.133	4.8	ng	437525	5	21.427	1836510	20.0
unknown24.233	24.233	51.5	ng	4992710	6	23.803	1937440	20.0
unknown28.215	28.215	72.3	ng	7008940	6	23.803	1937440	20.0