

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080323\
 Data File : BM041265.D
 Acq On : 03 Aug 2023 17:09
 Operator : MA/JU
 Sample : 03686-16
 Misc :
 ALS Vial : 10 Sample Multiplier: 2

Instrument :
 BNA_M
 ClientSampleId :
 SB-28-0-2-20230721

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: BM041265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	364	371	387	rBV	1876572	2736212	31.14%	4.424%
2	6.981	638	645	656	rBV	2004391	3126872	35.59%	5.056%
3	7.404	711	717	729	rBV2	47890	116497	1.33%	0.188%
4	7.793	777	783	792	rVB	1082962	1684079	19.17%	2.723%
5	8.975	975	984	995	rBV	1187219	2000854	22.77%	3.235%
6	10.604	1254	1261	1267	rBV	1641802	2625348	29.88%	4.245%
7	13.080	1674	1682	1694	rBV	3813204	5325659	60.61%	8.611%
8	13.351	1721	1728	1735	rBV	633540	982511	11.18%	1.589%
9	14.463	1908	1917	1924	rBV	2909998	4095585	46.61%	6.622%
10	14.886	1980	1989	1995	rBV4	35264	89838	1.02%	0.145%
11	15.963	2162	2172	2191	rBV	3389284	4811582	54.76%	7.780%
12	16.186	2203	2210	2217	rBV2	37943	96519	1.10%	0.156%
13	17.221	2380	2386	2391	rBV	3819712	5217621	59.38%	8.436%
14	17.262	2391	2393	2398	rVB	184744	223143	2.54%	0.361%
15	18.127	2532	2540	2549	rBV	2095431	3192517	36.33%	5.162%
16	18.415	2584	2589	2596	rBV3	50184	109986	1.25%	0.178%
17	18.662	2627	2631	2637	rBV2	57735	89152	1.01%	0.144%
18	19.039	2690	2695	2697	rBV2	74770	101671	1.16%	0.164%
19	19.068	2697	2700	2705	rVB2	156249	176463	2.01%	0.285%
20	19.286	2730	2737	2747	rBV	417482	727249	8.28%	1.176%
21	19.404	2753	2757	2771	rBV	1021558	1550813	17.65%	2.507%
22	19.621	2791	2794	2796	rBV2	96875	115600	1.32%	0.187%
23	19.651	2796	2799	2808	rVB	312544	455542	5.18%	0.737%
24	19.862	2829	2835	2840	rBV	7362614	8786434	100.00%	14.206%
25	20.156	2882	2885	2890	rVB2	138984	178890	2.04%	0.289%
26	20.656	2967	2970	2975	rVB	145271	155276	1.77%	0.251%
27	21.127	3046	3050	3058	rVB	679492	905844	10.31%	1.465%
28	21.427	3095	3101	3105	rBV	4281154	5404475	61.51%	8.738%
29	21.568	3122	3125	3135	rVB2	192685	245724	2.80%	0.397%
30	22.021	3199	3202	3205	rBV	179716	196127	2.23%	0.317%
31	22.421	3266	3270	3278	rVB	413308	627473	7.14%	1.015%
32	23.056	3374	3378	3383	rBV2	269915	467642	5.32%	0.756%
33	23.803	3498	3505	3513	rBV	2403958	4501028	51.23%	7.278%
34	24.368	3597	3601	3608	rVB	396843	727885	8.28%	1.177%

Sum of corrected areas: 61848111

Instrument :

BNA_M

ClientSampleId :

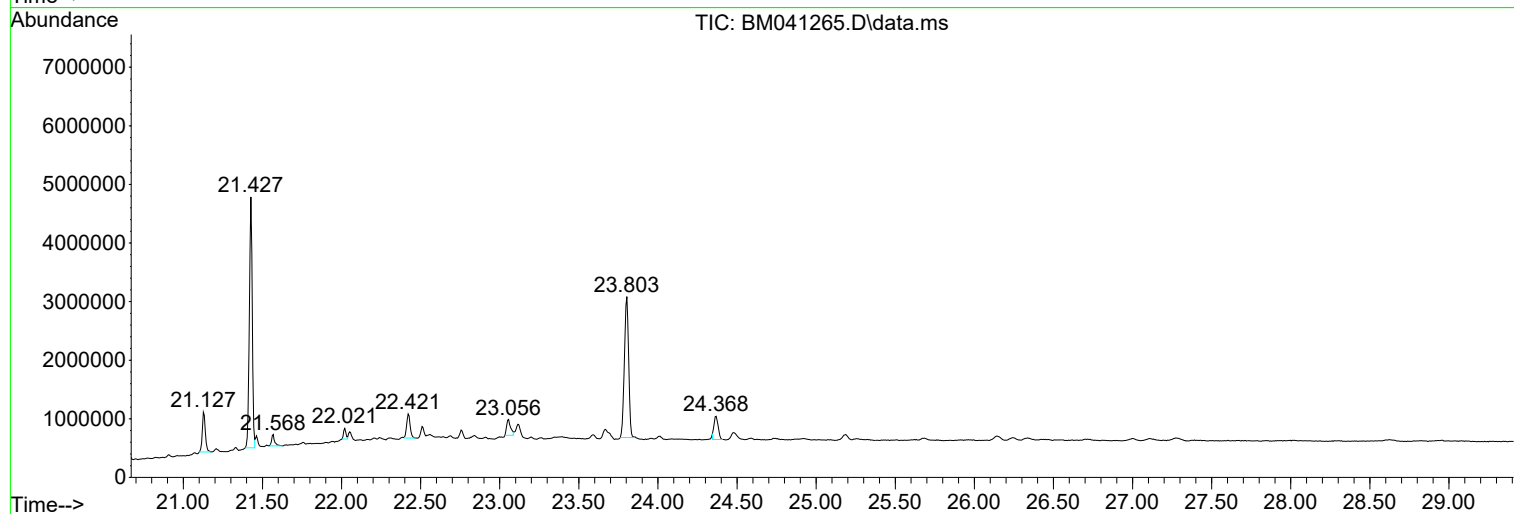
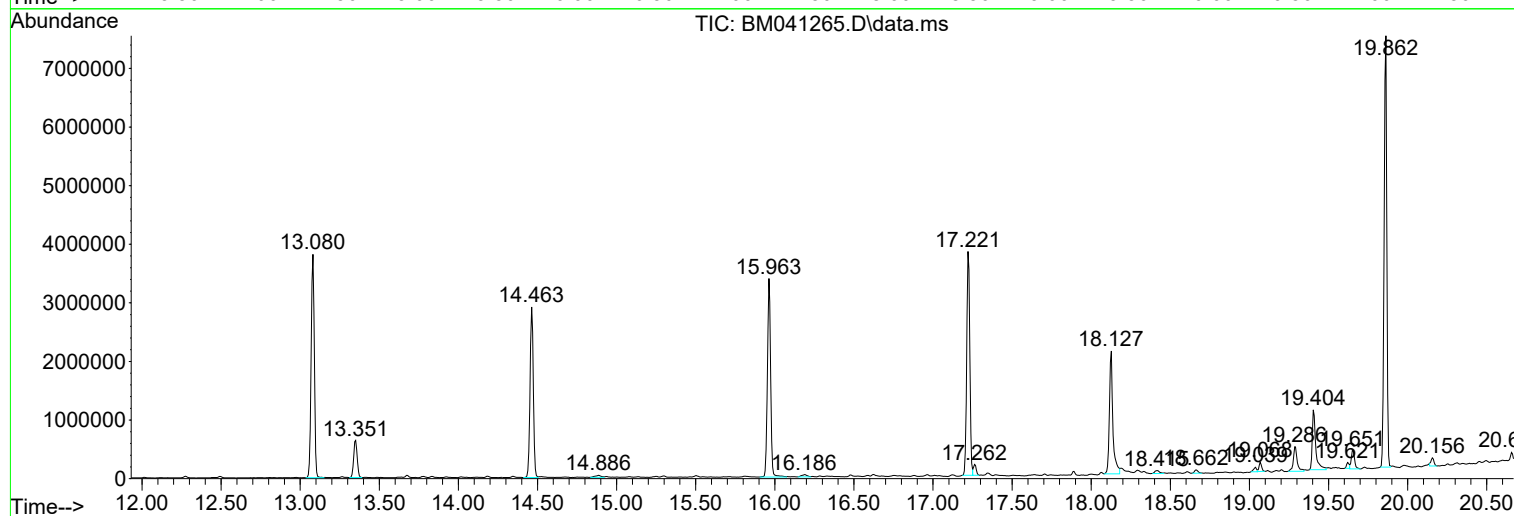
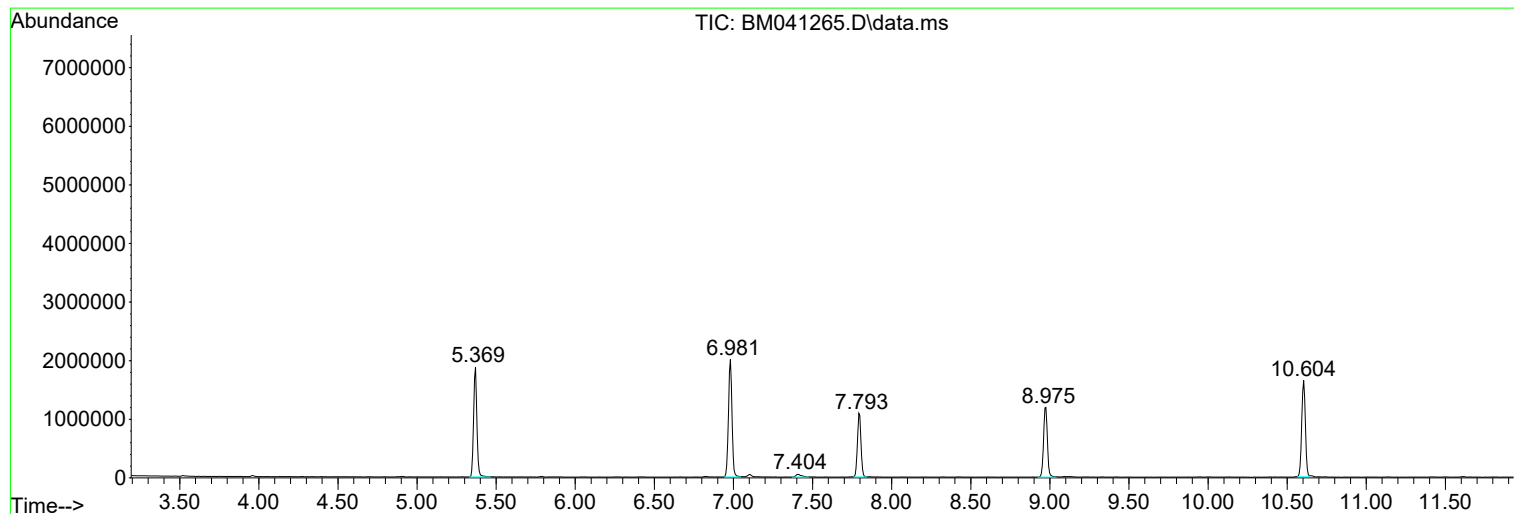
SB-28-0-2-20230721

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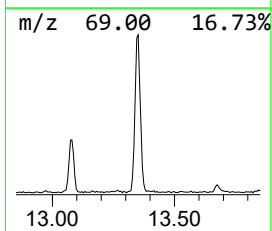
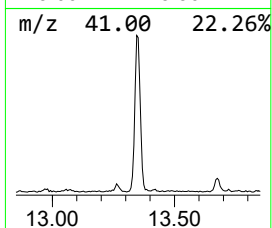
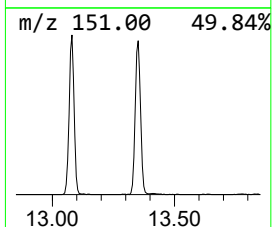
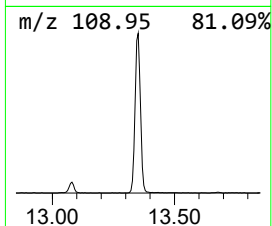
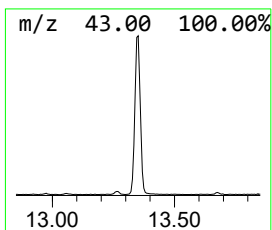
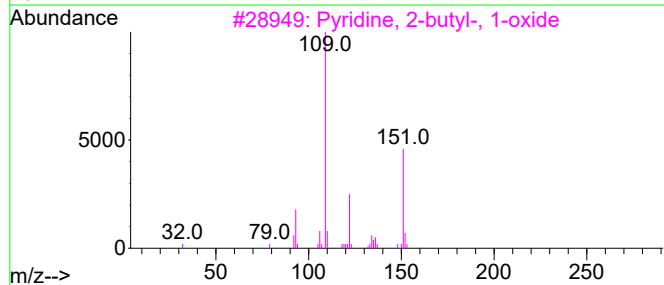
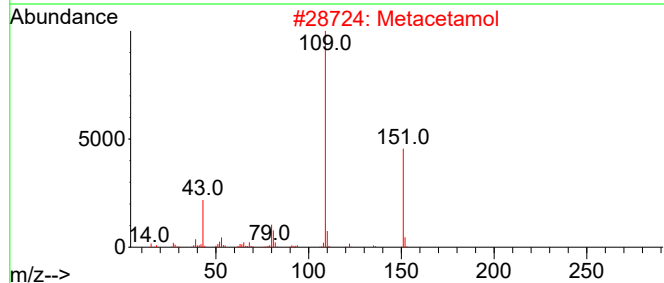
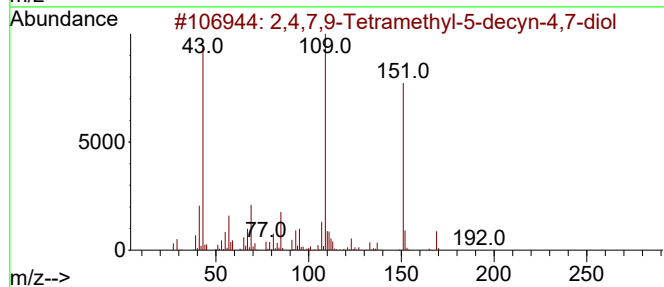
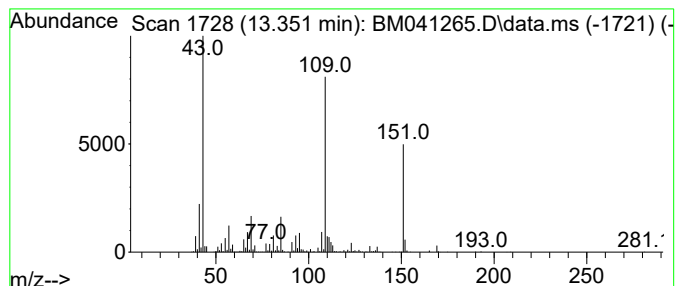
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	4.80 ng	982511	Acenaphthene-d10	14.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	64	
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
4	Acetaminophen	151	C8H9NO2	000103-90-2	59	
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59	



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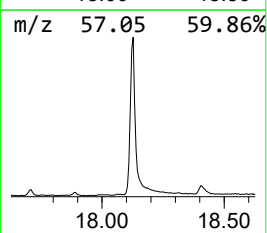
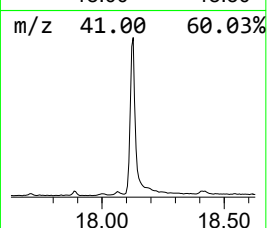
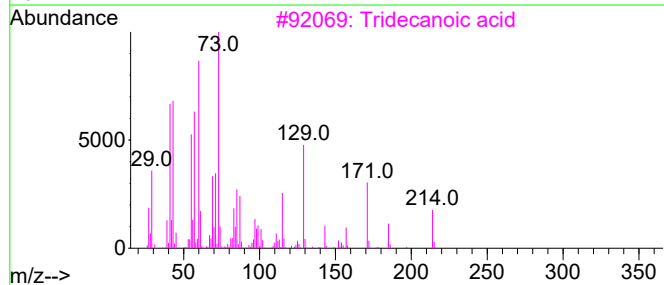
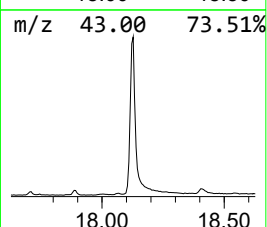
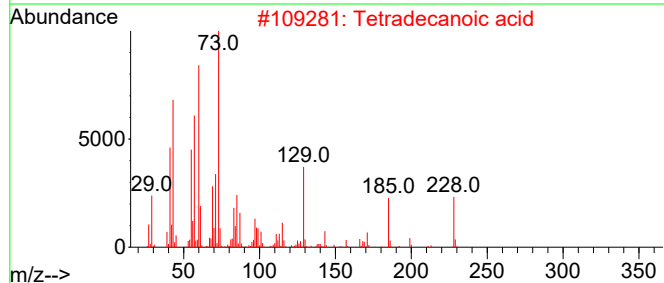
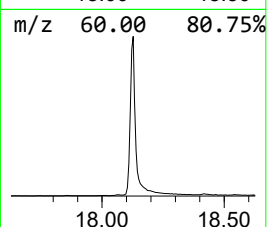
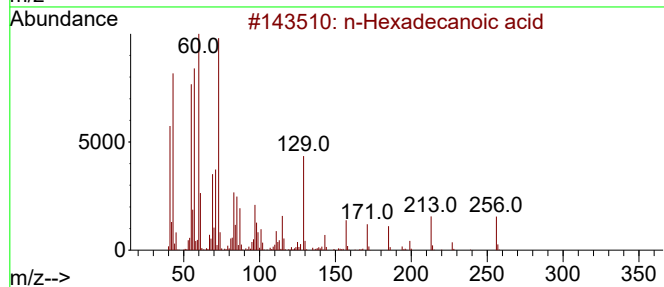
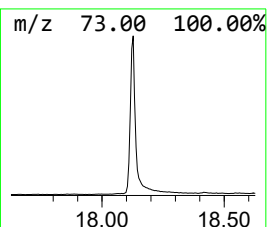
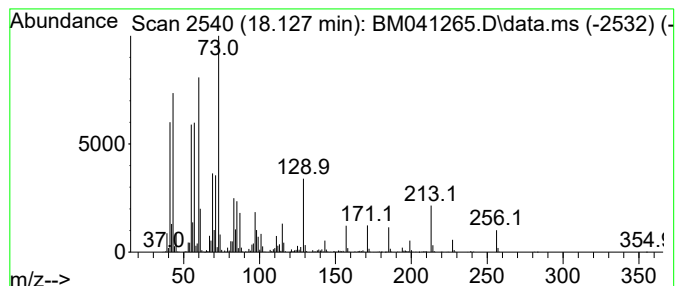
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	12.24 ng	3192520	Phenanthrene-d10	17.221

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	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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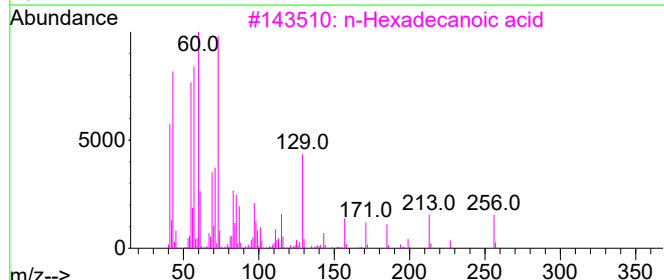
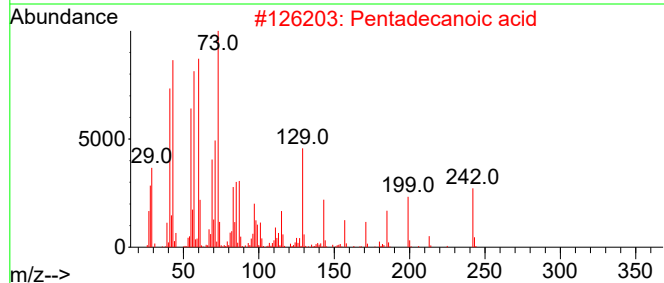
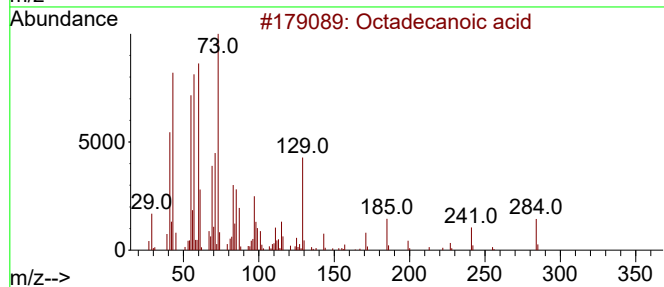
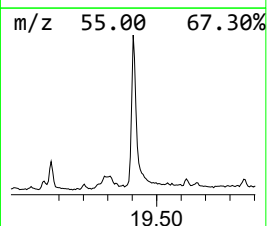
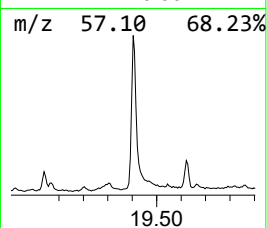
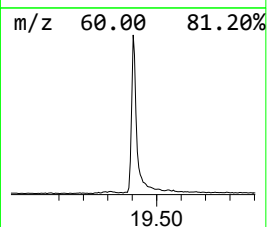
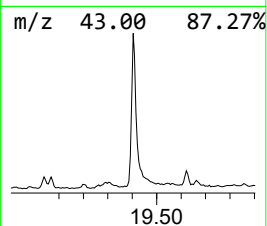
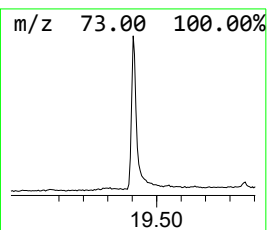
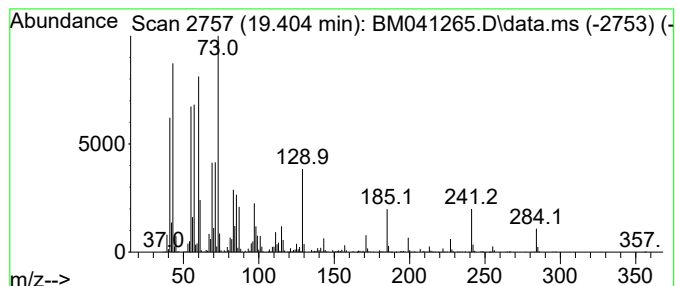
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	5.74 ng	1550810	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	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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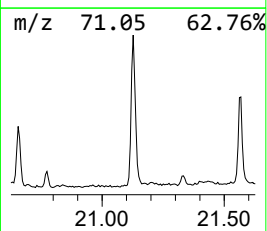
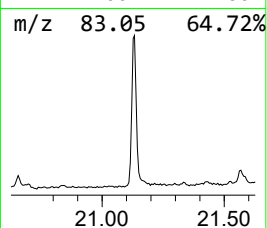
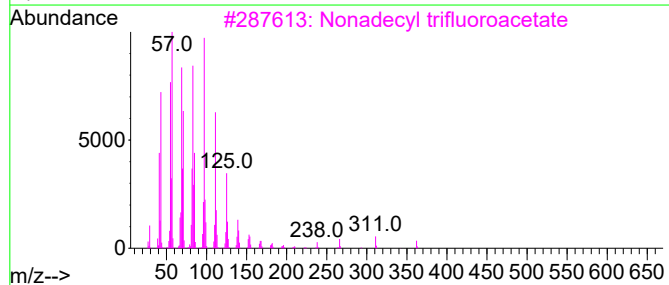
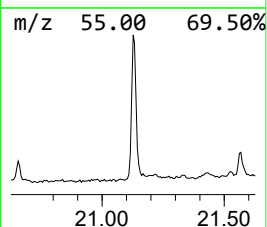
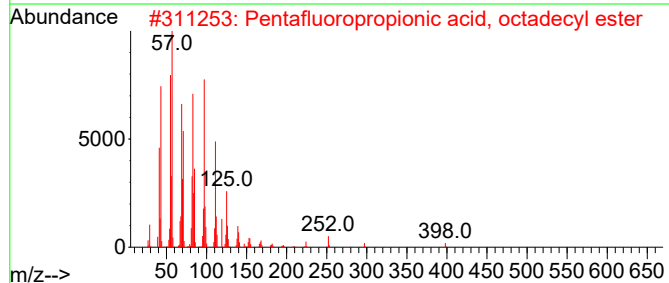
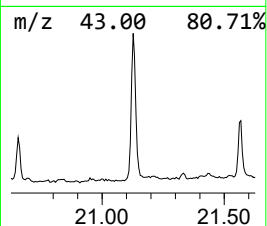
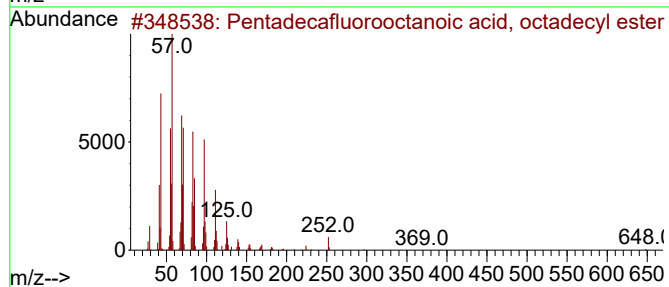
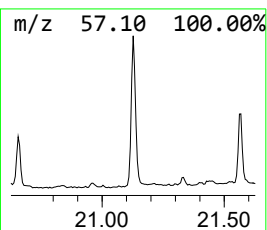
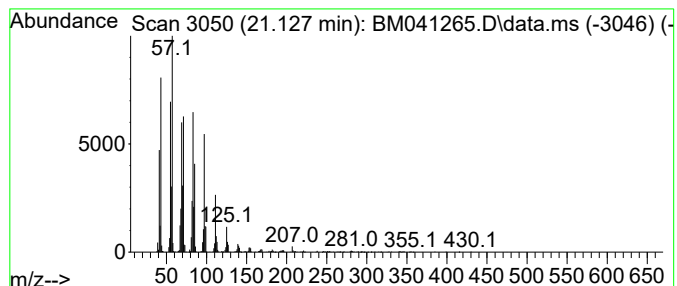
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	3.35 ng	905844	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	86
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81



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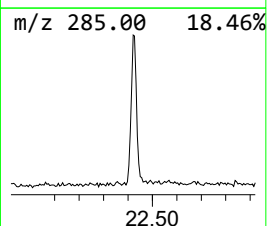
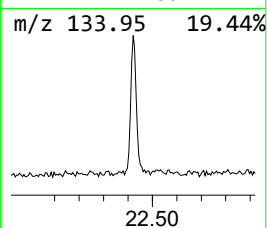
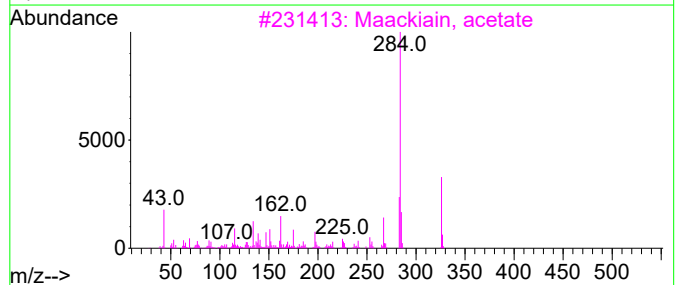
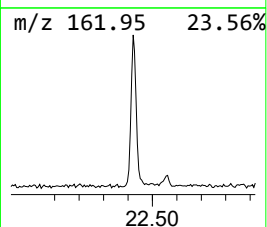
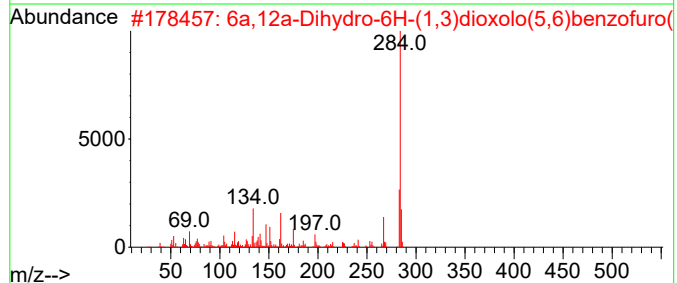
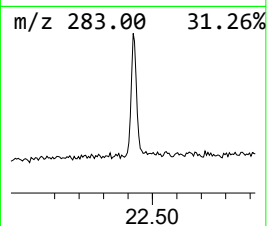
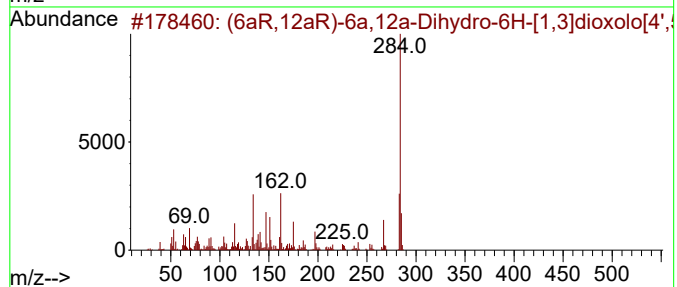
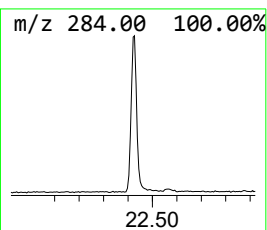
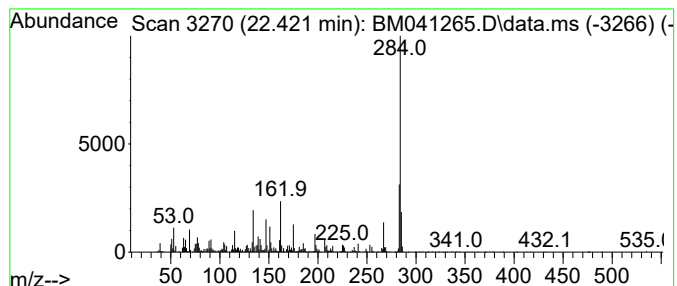
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (6aR,12aR)-6a,12a-Dihydro-6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.421	2.32 ng	627473	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(6aR,12aR)-6a,12a-Dihydro-6H-[1,...	284	C16H12O5	002035-15-6	96
2			6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	076496-57-6	94
3			Maackiain, acetate	326	C18H14O6	002035-16-7	68
4			Homopterocarpin	284	C17H16O4	000606-91-7	60
5			4-Amino-5-(4-nitrophenylazo)benz...	284	C12H8N6O3	166766-07-0	58



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ClientSampleId :
SB-28-0-2-20230721

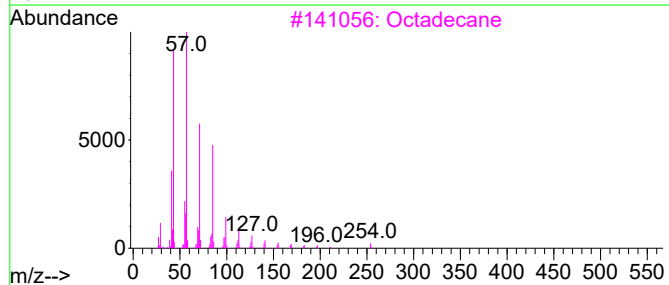
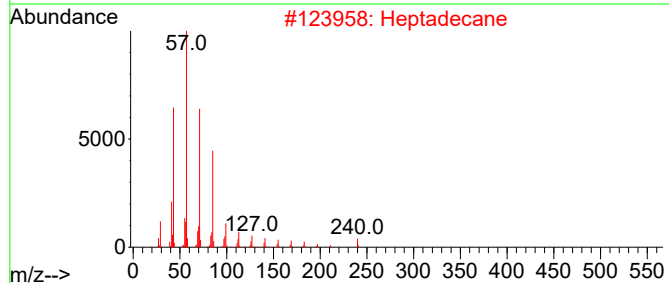
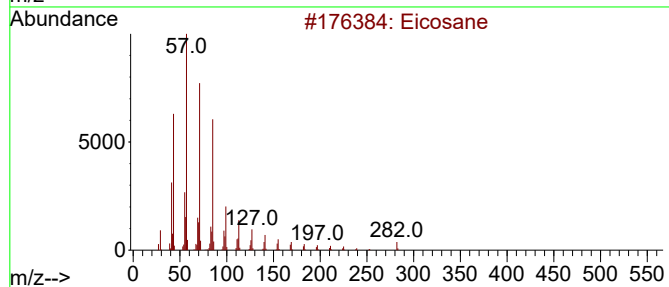
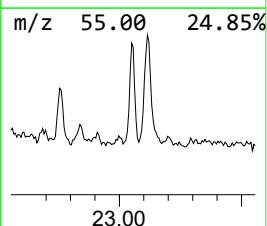
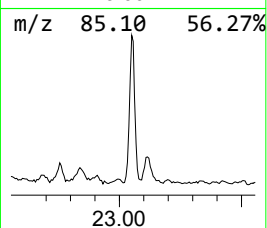
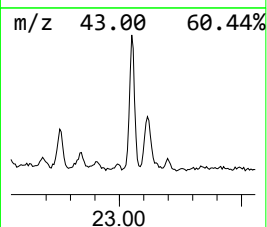
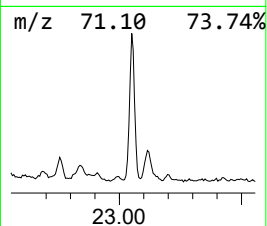
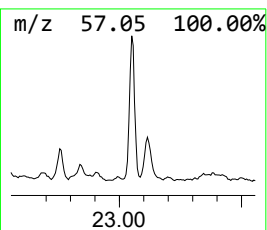
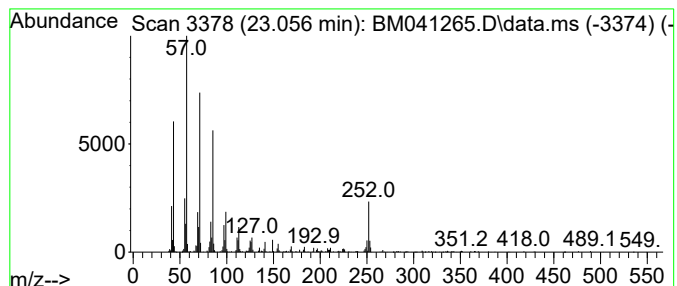
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.056	2.08 ng	467642	Perylene-d12	23.803

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Heptadecane	240	C17H36	000629-78-7	94
3			Octadecane	254	C18H38	000593-45-3	93
4			Hexacosane	366	C26H54	000630-01-3	93
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080323\
Data File : BM041265.D
Acq On : 03 Aug 2023 17:09
Operator : MA/JU
Sample : 03686-16
Misc :
ALS Vial : 10 Sample Multiplier: 2

Instrument :
BNA_M
ClientSampleId :
SB-28-0-2-20230721

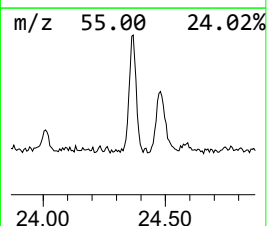
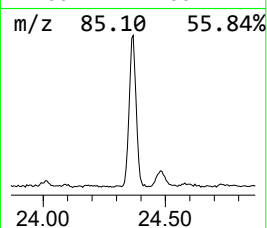
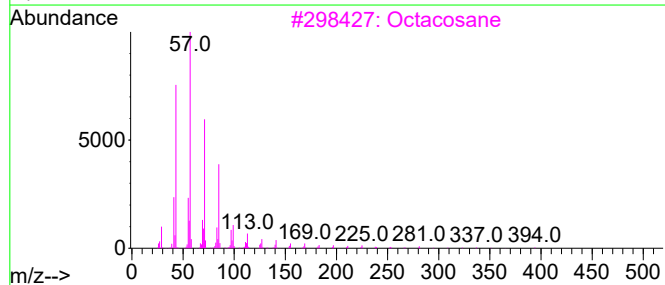
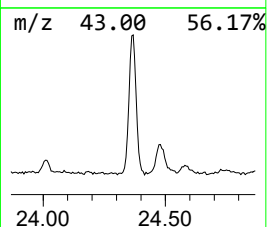
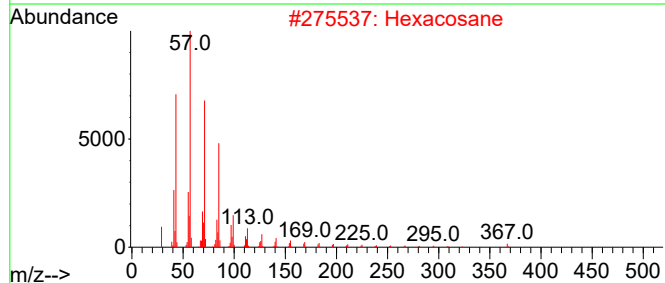
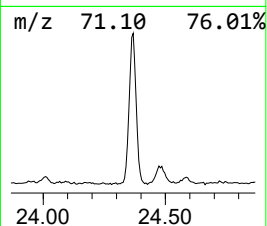
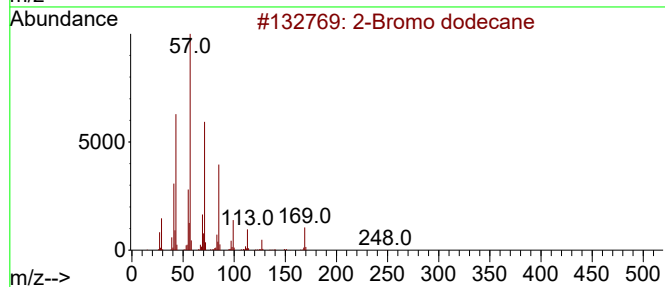
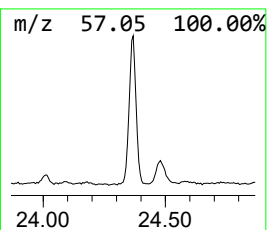
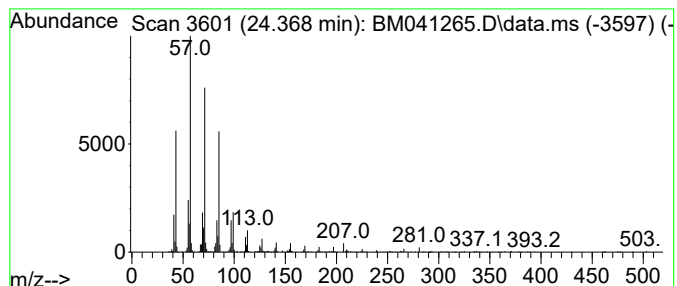
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.368	3.23 ng	727885	Perylene-d12	23.803

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080323\
Data File : BM041265.D
Acq On : 03 Aug 2023 17:09
Operator : MA/JU
Sample : 03686-16
Misc :
ALS Vial : 10 Sample Multiplier: 2

Instrument :
BNA_M
ClientSampleId :
SB-28-0-2-20230721

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
2,4,7,9-Tetrame...	13.351	4.8	ng	982511	3	14.463	4095590	20.0
n-Hexadecanoic ...	18.127	12.2	ng	3192520	4	17.221	5217620	20.0
Octadecanoic acid	19.404	5.7	ng	1550810	5	21.427	5404480	20.0
Pentadecafluoro...	21.127	3.4	ng	905844	5	21.427	5404480	20.0
(6aR,12aR)-6a,1...	22.421	2.3	ng	627473	5	21.427	5404480	20.0
Eicosane	23.056	2.1	ng	467642	6	23.803	4501030	20.0
2-Bromo dodecane	24.368	3.2	ng	727885	6	23.803	4501030	20.0