

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
 Data File : BM036096.D
 Acq On : 04 Aug 2022 13:28
 Operator : CG/JU
 Sample : N3935-14
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-144

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036096.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	404	rBV	6514449	9212414	43.19%	7.766%
2	7.034	659	671	684	rBV	6156268	9966735	46.72%	8.402%
3	7.857	800	811	820	rBV	1323404	2072351	9.71%	1.747%
4	9.028	1002	1010	1017	rBV	3902557	6375673	29.89%	5.375%
5	10.663	1278	1288	1294	rBV	1883565	3128764	14.67%	2.638%
6	12.327	1564	1571	1579	rVB	195221	338595	1.59%	0.285%
7	12.545	1602	1608	1614	rBV	170442	264523	1.24%	0.223%
8	13.127	1700	1707	1717	rBV	10398352	14762537	69.20%	12.445%
9	13.821	1820	1825	1830	rBV	140860	223265	1.05%	0.188%
10	14.498	1932	1940	1946	rBV	2927370	4165650	19.53%	3.512%
11	14.915	2003	2011	2015	rBV3	150088	355592	1.67%	0.300%
12	15.751	2148	2153	2160	rVB	216140	454986	2.13%	0.384%
13	15.986	2186	2193	2200	rBV	8459225	11691010	54.81%	9.856%
14	16.210	2226	2231	2233	rBV2	217948	325795	1.53%	0.275%
15	16.645	2301	2305	2312	rVB3	147246	237768	1.11%	0.200%
16	16.998	2361	2365	2370	rVB	232012	257678	1.21%	0.217%
17	17.139	2385	2389	2396	rBV2	158496	269176	1.26%	0.227%
18	17.239	2401	2406	2411	rVV	3552295	4905260	23.00%	4.135%
19	17.280	2411	2413	2418	rVB	292278	338706	1.59%	0.286%
20	17.739	2487	2491	2496	rBV	261691	312854	1.47%	0.264%
21	17.915	2517	2521	2526	rVB	315977	362044	1.70%	0.305%
22	18.145	2552	2560	2574	rBV2	2791592	4455984	20.89%	3.756%
23	18.433	2604	2609	2613	rBV	377565	524125	2.46%	0.442%
24	19.068	2714	2717	2718	rVV	272592	306352	1.44%	0.258%
25	19.086	2718	2720	2724	rVB2	323875	361108	1.69%	0.304%
26	19.298	2752	2756	2764	rVB2	629420	841259	3.94%	0.709%
27	19.421	2773	2777	2785	rVB	853424	1129991	5.30%	0.953%
28	19.650	2812	2816	2826	rVB2	407962	848190	3.98%	0.715%
29	19.868	2847	2853	2858	rBV	17343516	21331665	100.00%	17.983%
30	20.156	2899	2902	2904	rBV2	192007	249357	1.17%	0.210%
31	20.674	2986	2990	2993	rVB2	297219	337771	1.58%	0.285%
32	21.139	3065	3069	3077	rBV	2444820	3148204	14.76%	2.654%
33	21.421	3112	3117	3121	rBV	4142486	5358636	25.12%	4.517%
34	21.580	3141	3144	3152	rBV3	255515	384103	1.80%	0.324%
35	22.033	3218	3221	3223	rBV	281812	375531	1.76%	0.317%
36	23.068	3393	3397	3402	rVB	373845	555163	2.60%	0.468%

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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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.785	3513	3519	3526	rVB	2056202	3917328	18.36%	3.302%
38	26.491	3971	3979	3992	rVB2	1483941	4476690	20.99%	3.774%

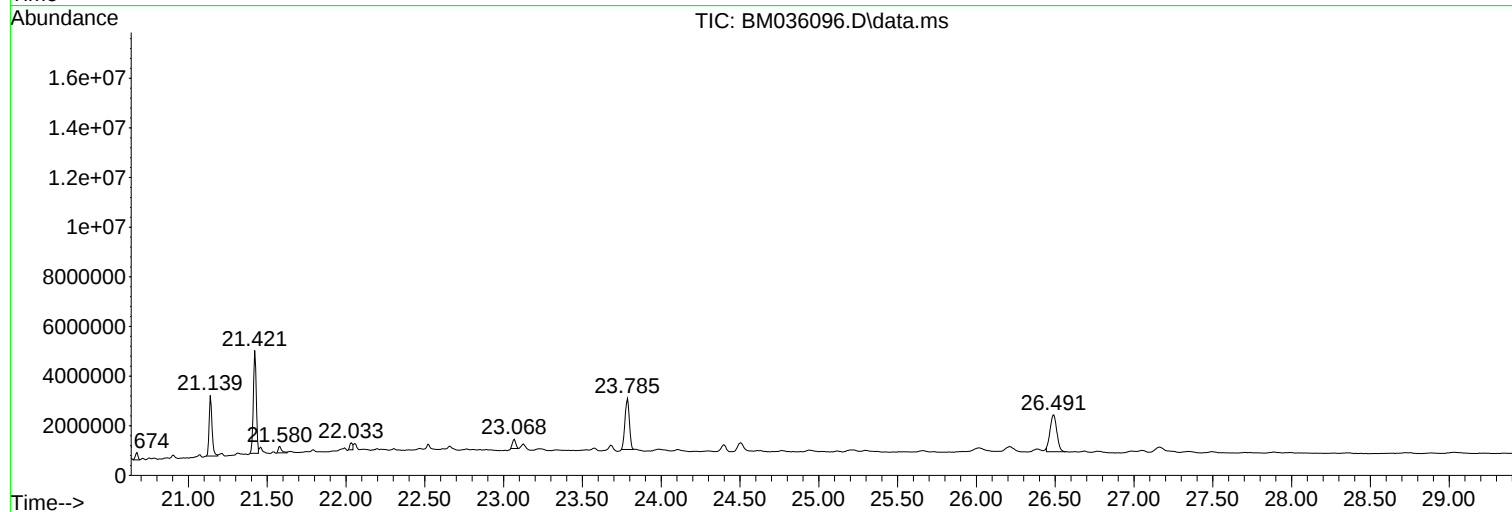
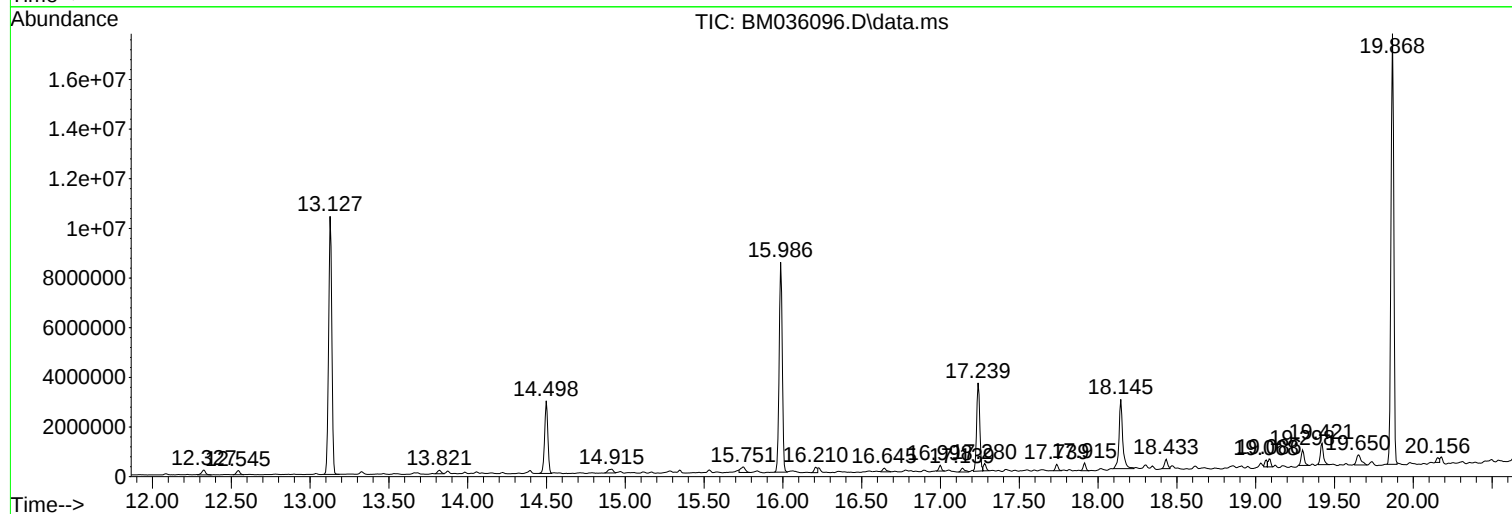
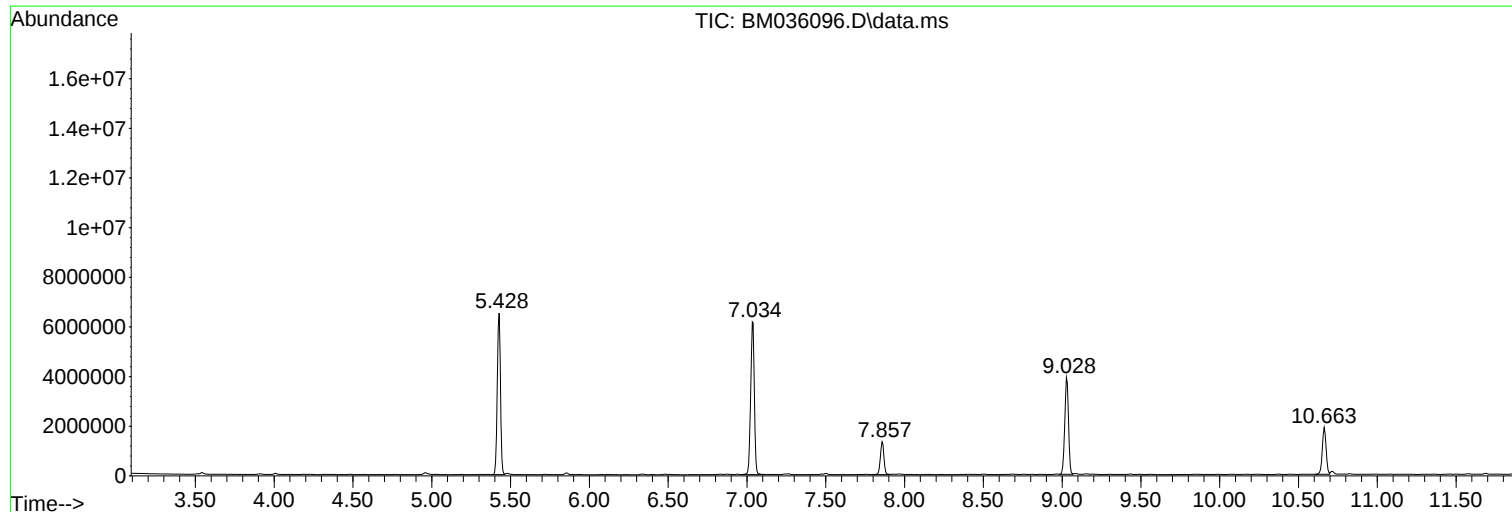
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 5 Sample Multiplier: 1

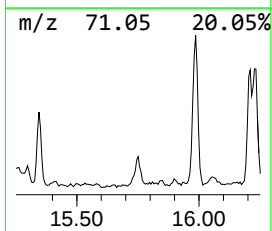
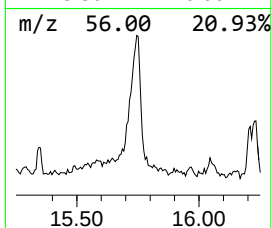
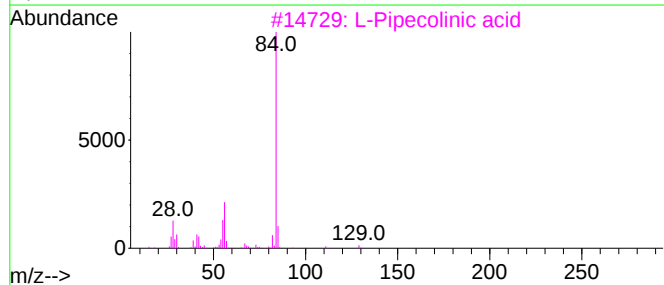
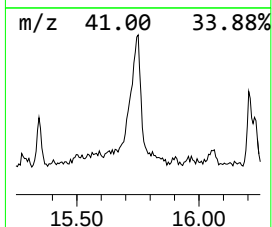
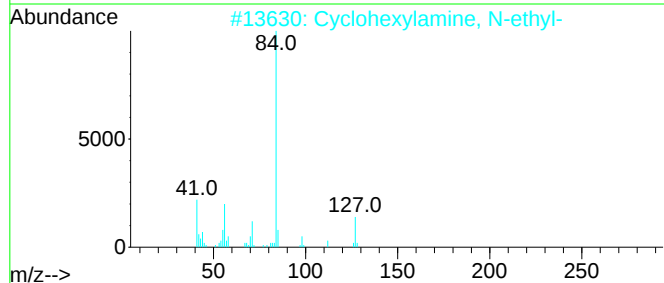
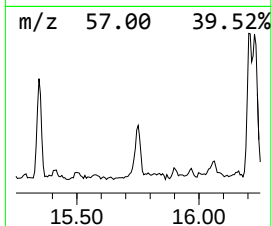
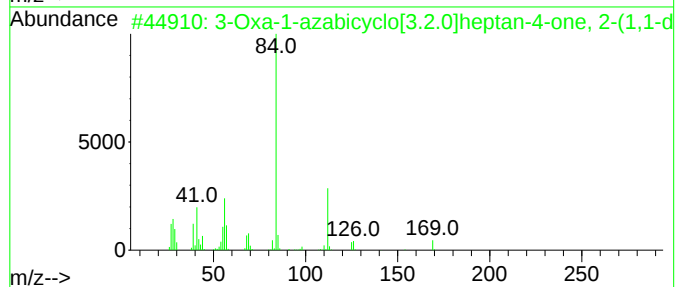
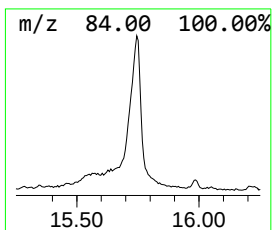
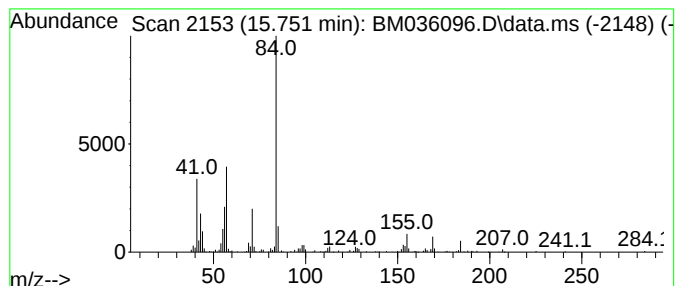
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Oxa-1-azabicyclo[3.2.0]he... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.751	2.18 ng	454986	Acenaphthene-d10		14.498
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Oxa-1-azabicyclo[3.2.0]heptan-...	169	C9H15NO2	086046-39-1	59
2	Cyclohexylamine, N-ethyl-	127	C8H17N	005459-93-8	59
3	L-Pipecolic acid	129	C6H11NO2	003105-95-1	58
4	Boc-Pyr-OH, methyl ester	243	C11H17NO5	108963-96-8	53
5	2-Piperidinemethanol	115	C6H13NO	003433-37-2	53



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-144

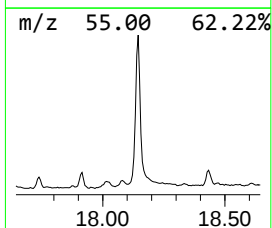
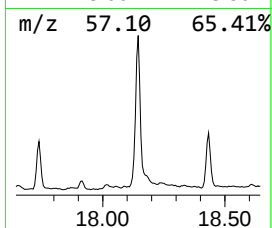
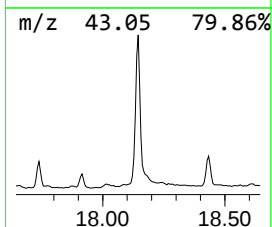
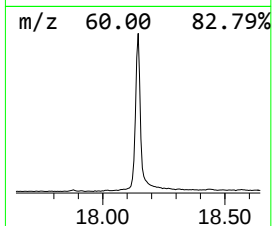
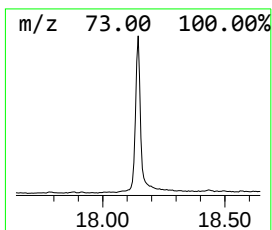
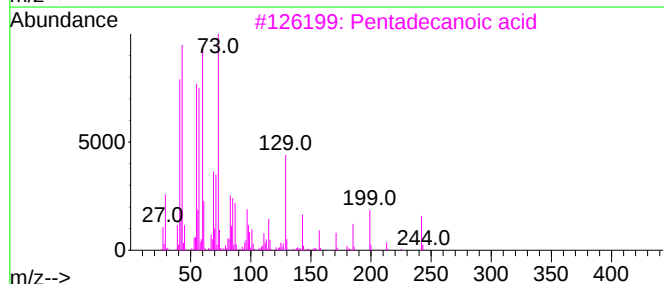
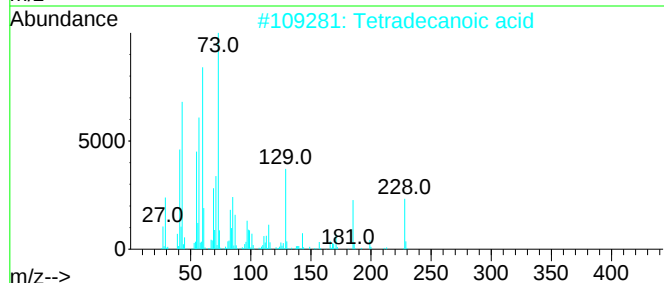
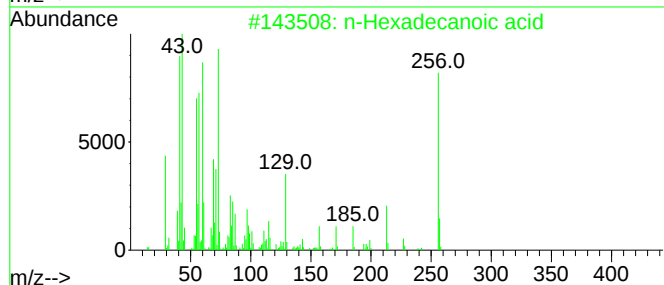
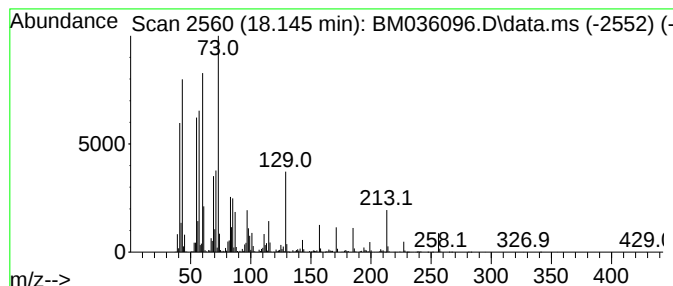
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	18.17 ng	4455980	Phenanthrene-d10	17.239

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



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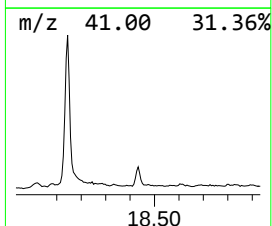
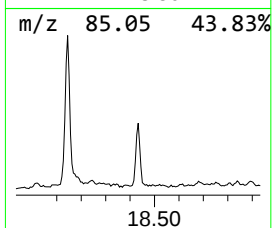
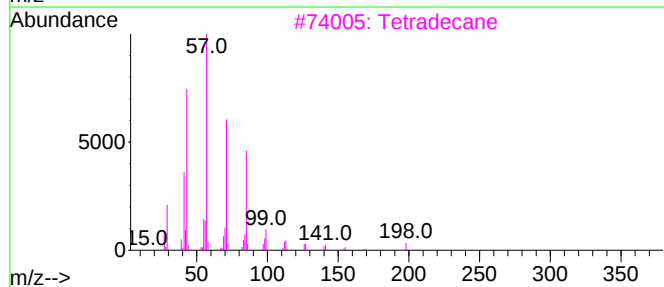
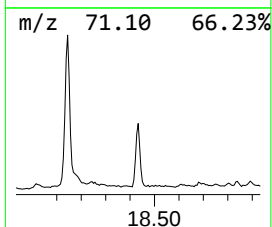
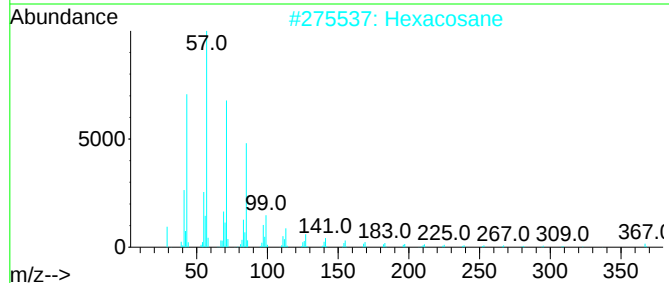
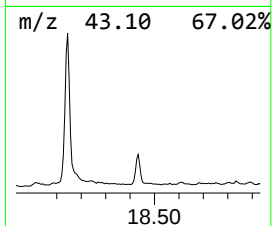
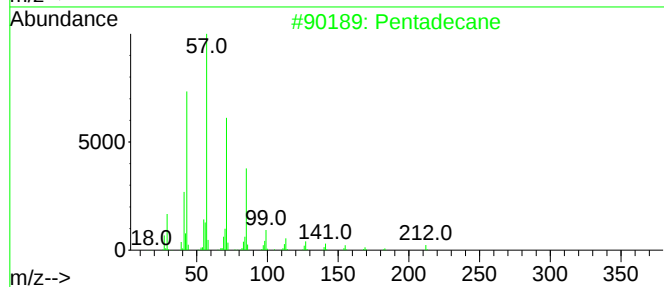
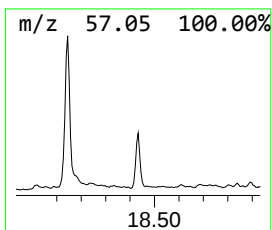
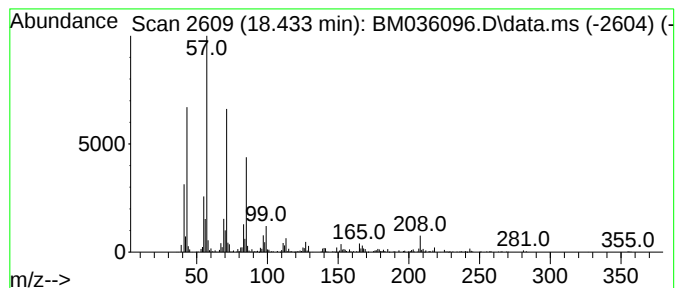
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.433	2.14 ng	524125	Phenanthrene-d10	17.239

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane	212	C15H32	000629-62-9	91
2		Hexacosane	366	C26H54	000630-01-3	87
3		Tetradecane	198	C14H30	000629-59-4	83
4		Tetracosane	338	C24H50	000646-31-1	83
5		Heptacosane	380	C27H56	000593-49-7	83



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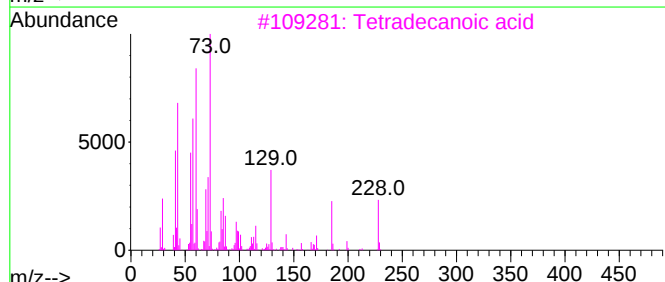
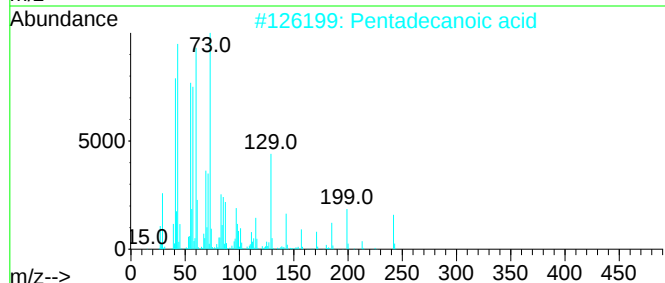
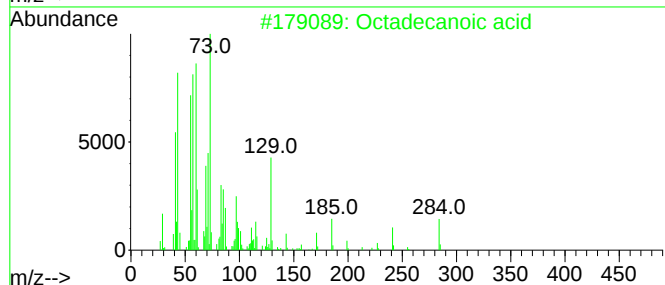
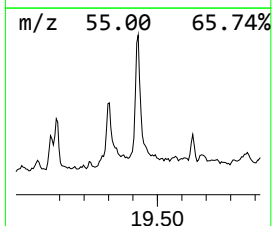
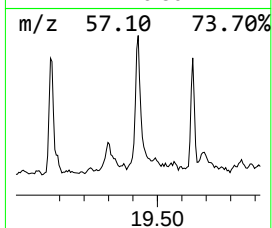
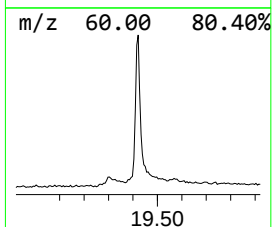
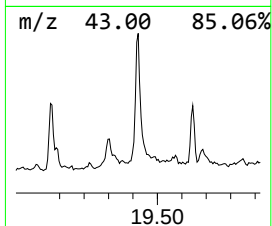
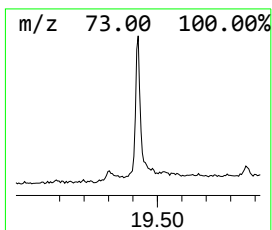
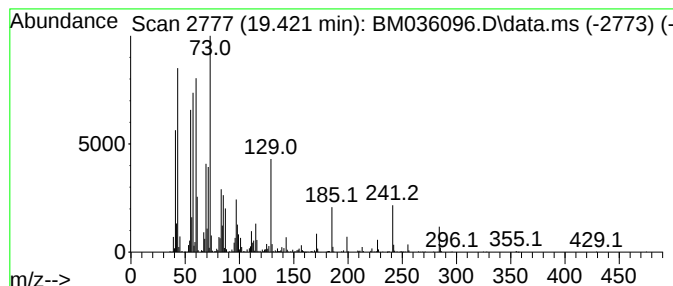
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.421	4.22 ng	1129990	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	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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ClientSampleId :
RVE-144

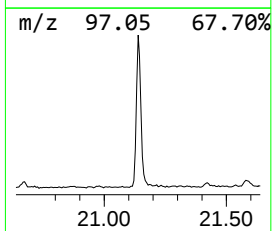
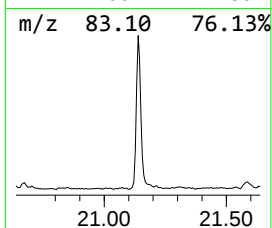
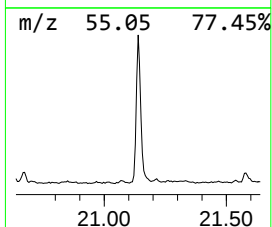
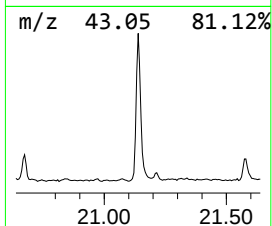
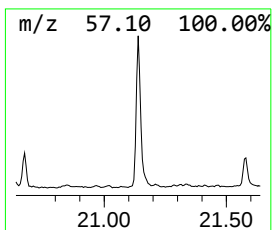
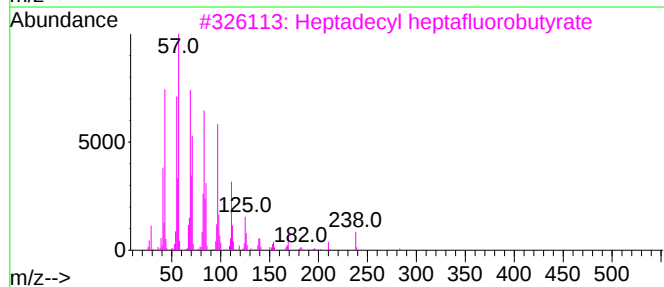
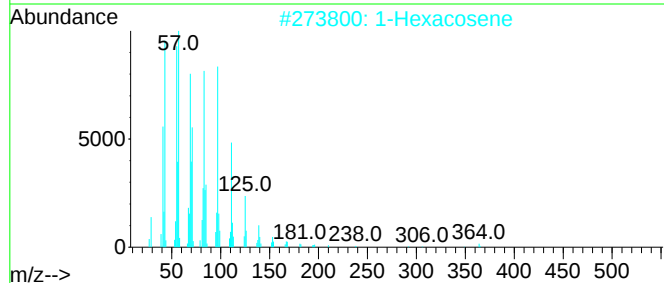
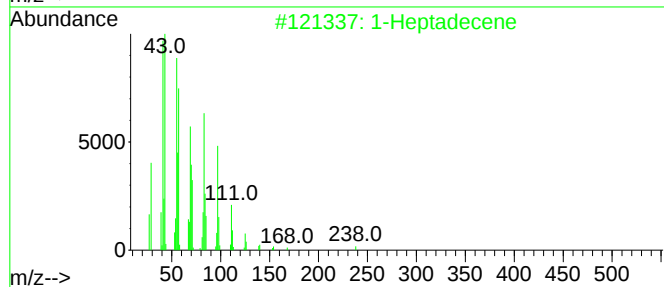
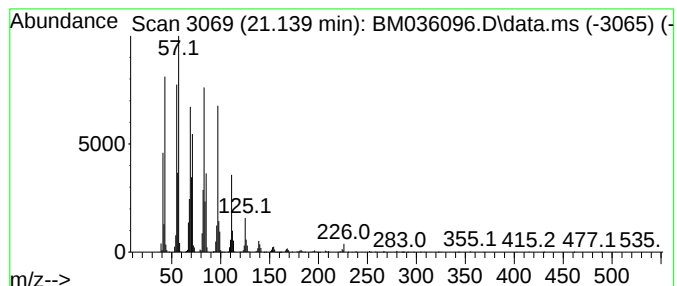
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heptadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	11.75 ng	3148200	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	94
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036096.D
Acq On : 04 Aug 2022 13:28
Operator : CG/JU
Sample : N3935-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-144

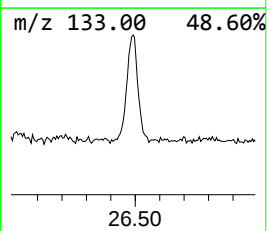
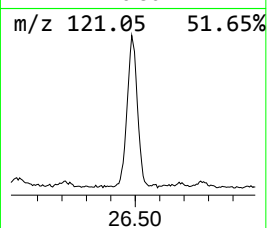
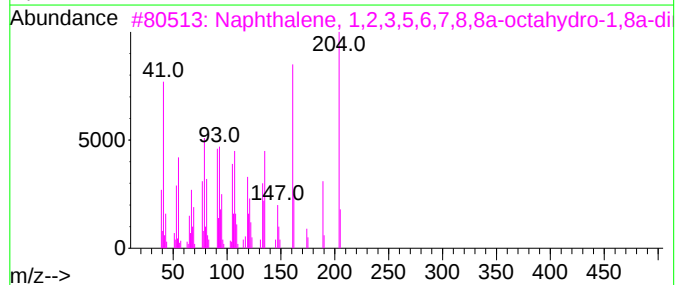
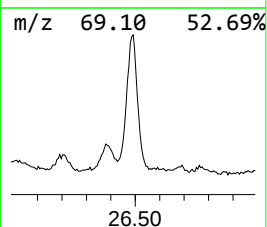
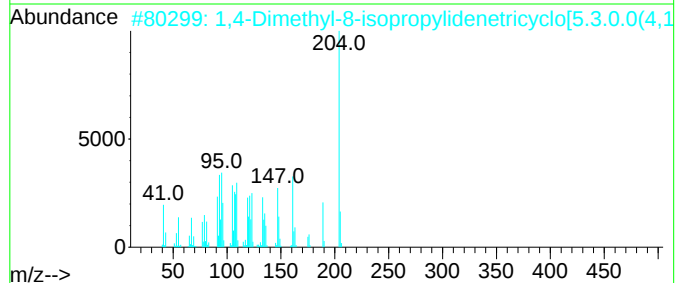
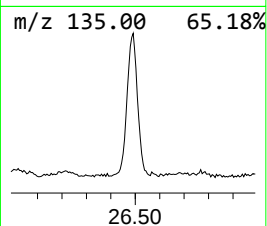
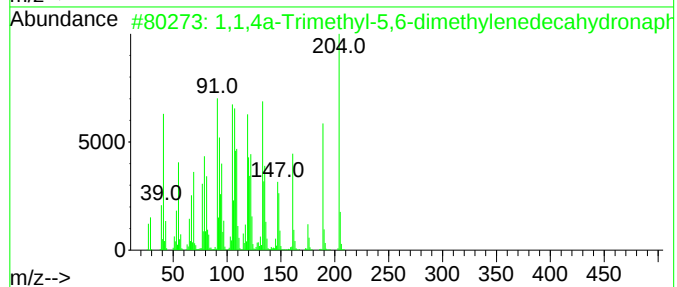
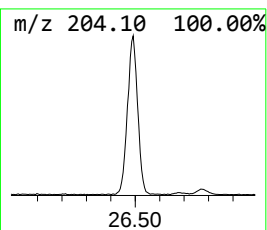
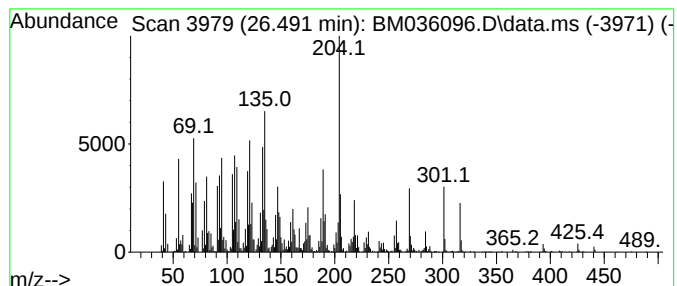
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.491	22.86 ng	4476690	Perylene-d12	23.785

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	58		
2	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	58		
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	50		
4	Farnesyl bromide	284	C15H25Br	006874-67-5	49		
5	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	46		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036096.D
Acq On : 04 Aug 2022 13:28
Operator : CG/JU
Sample : N3935-14
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-144

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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
3-Oxa-1-azabicy...	15.751	2.2	ng	454986	3	14.498	4165650	20.0
n-Hexadecanoic ...	18.145	18.2	ng	4455980	4	17.239	4905260	20.0
Pentadecane	18.433	2.1	ng	524125	4	17.239	4905260	20.0
Octadecanoic acid	19.421	4.2	ng	1129990	5	21.421	5358640	20.0
1-Heptadecene	21.139	11.8	ng	3148200	5	21.421	5358640	20.0
1,1,4a-Trimethy...	26.491	22.9	ng	4476690	6	23.785	3917330	20.0