

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
 Data File : BF134311.D
 Acq On : 15 Jul 2023 03:09
 Operator : CG\JU
 Sample : 03597-09
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-46-(0-2)

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_F\Methods\8270-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	506	509	518	rVB	20256	27219	1.69%	0.215%
2	5.469	572	575	588	rBV	1423075	1460242	90.55%	11.523%
3	6.475	742	746	764	rBV	1462316	1525451	94.60%	12.037%
4	6.675	776	780	795	rBV	22248	41893	2.60%	0.331%
5	6.839	805	808	816	rBV	633767	504958	31.31%	3.985%
6	7.404	900	904	907	rBV	1168223	947221	58.74%	7.475%
7	8.122	1022	1026	1037	rBV	705890	647383	40.15%	5.108%
8	9.198	1205	1209	1212	rBV	1961227	1612611	100.00%	12.725%
9	9.310	1225	1228	1231	rBV	23766	20157	1.25%	0.159%
10	9.880	1321	1325	1328	rBV	760384	679404	42.13%	5.361%
11	10.674	1456	1460	1472	rBV	1149474	1141058	70.76%	9.004%
12	11.374	1575	1579	1582	rBV	768174	681456	42.26%	5.377%
13	11.398	1582	1583	1586	rVV	46959	29265	1.81%	0.231%
14	11.439	1588	1590	1595	rVB3	18149	18645	1.16%	0.147%
15	11.904	1666	1669	1676	rBV	156063	161547	10.02%	1.275%
16	12.592	1783	1786	1790	rBV	70848	75250	4.67%	0.594%
17	12.692	1799	1803	1807	rBV2	37132	43265	2.68%	0.341%
18	12.827	1821	1826	1830	rVB	61201	67098	4.16%	0.529%
19	12.968	1846	1850	1853	rBV	1587394	1298256	80.51%	10.245%
20	13.910	2006	2010	2021	rVB6	31364	77046	4.78%	0.608%
21	14.033	2024	2031	2034	rBV	600385	585051	36.28%	4.617%
22	14.057	2034	2035	2043	rVB	41064	40768	2.53%	0.322%
23	14.504	2107	2111	2115	rBV	36541	39105	2.42%	0.309%
24	14.815	2160	2164	2169	rVB4	14948	19794	1.23%	0.156%
25	15.098	2207	2212	2215	rBV3	24347	41986	2.60%	0.331%
26	15.168	2220	2224	2228	rVB	44756	52994	3.29%	0.418%
27	15.409	2262	2265	2272	rVB	15741	18759	1.16%	0.148%
28	15.474	2272	2276	2281	rVB	20037	27358	1.70%	0.216%
29	15.539	2282	2287	2299	rBV	312214	432331	26.81%	3.412%
30	15.774	2324	2327	2334	rVB4	30035	44934	2.79%	0.355%
31	16.021	2364	2369	2375	rVB2	39906	59796	3.71%	0.472%
32	16.504	2446	2451	2452	rBV5	21145	32692	2.03%	0.258%
33	16.868	2509	2513	2519	rVB5	22267	40673	2.52%	0.321%
34	17.186	2561	2567	2573	rBV10	14945	35974	2.23%	0.284%
35	17.909	2683	2690	2702	rVB6	44066	119315	7.40%	0.942%
36	18.262	2745	2750	2751	rBV5	14150	21714	1.35%	0.171%

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RB-46-(0-2)

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_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

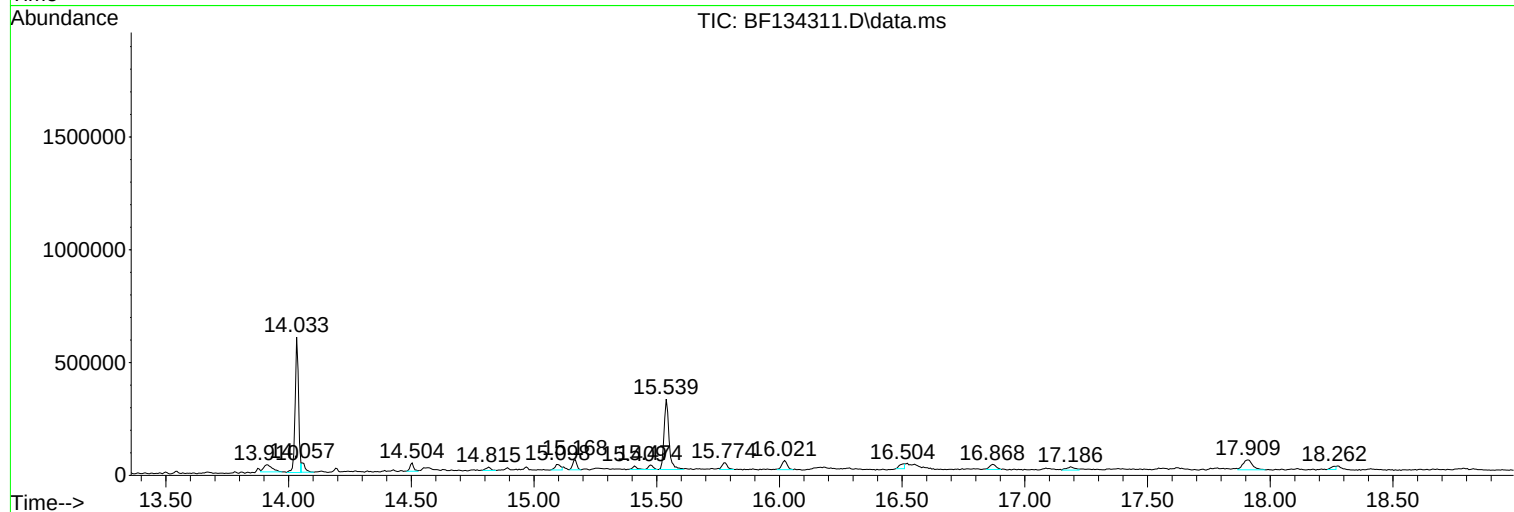
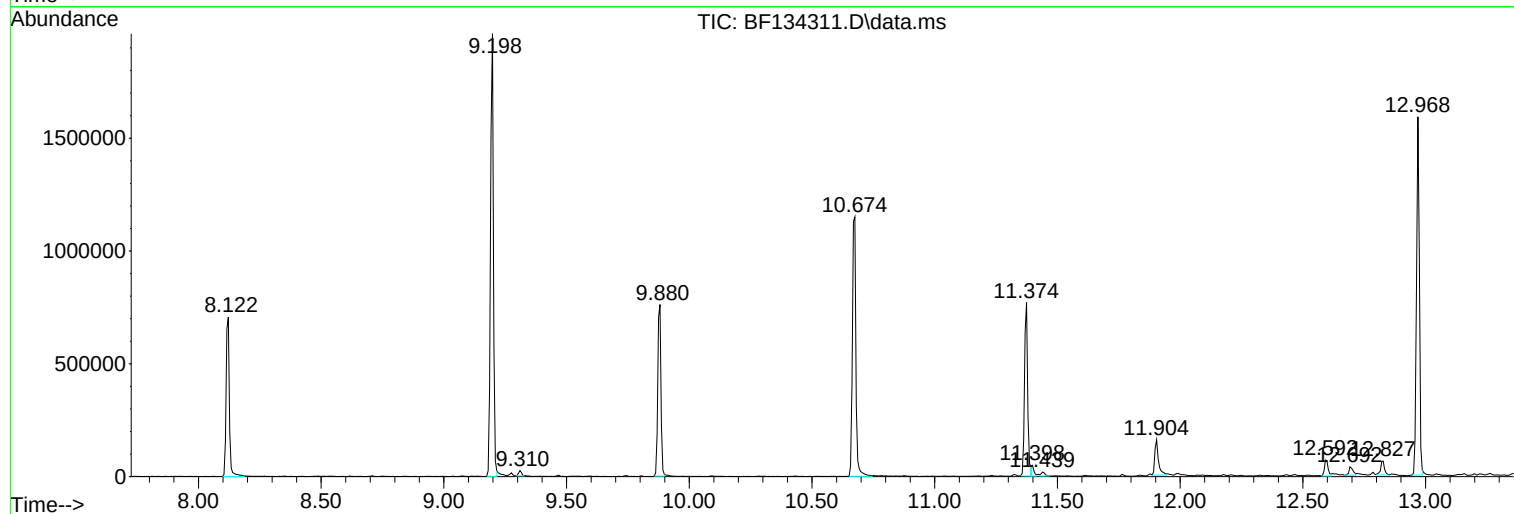
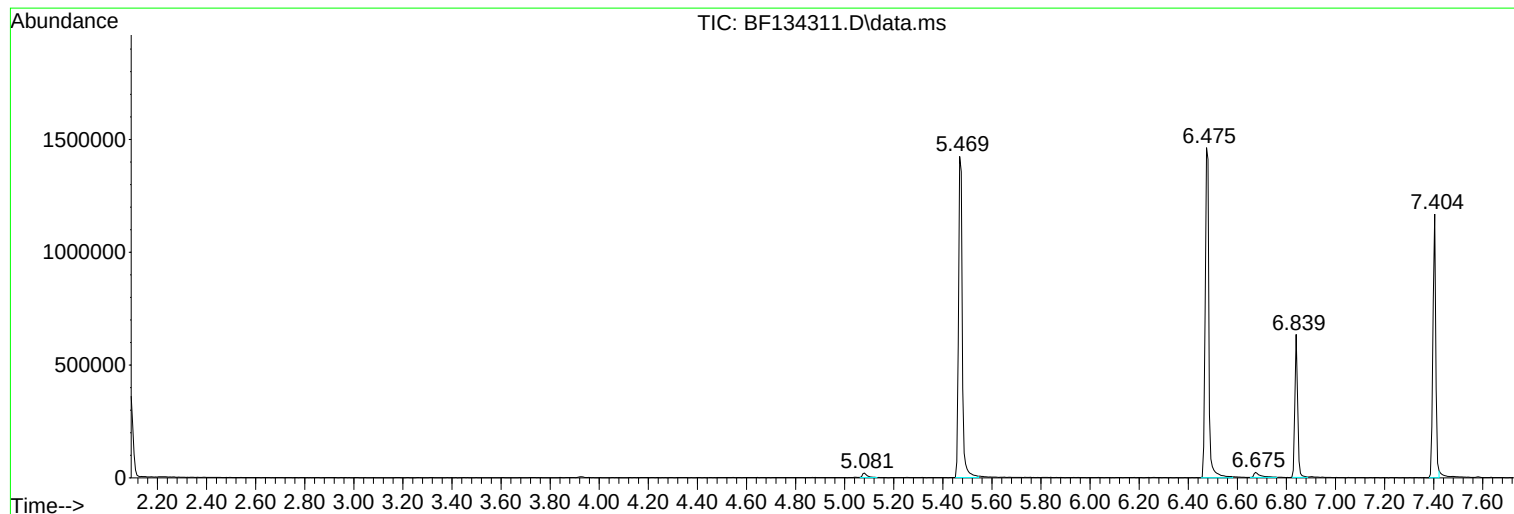
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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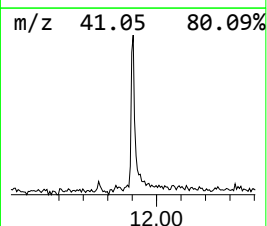
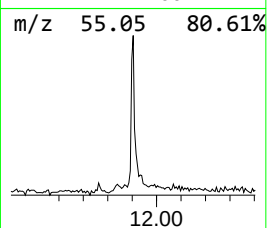
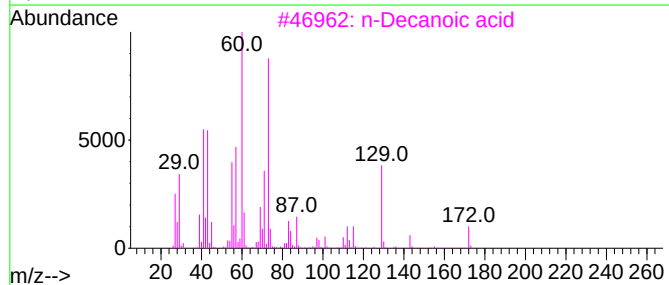
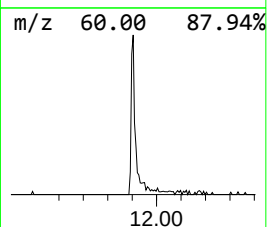
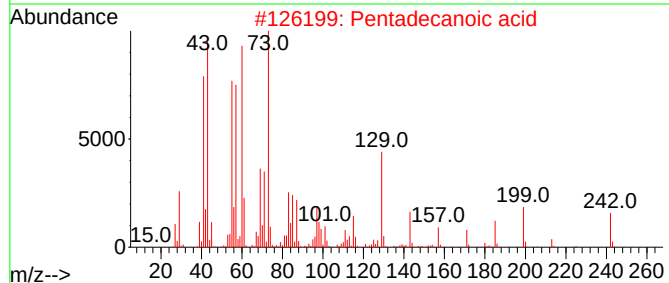
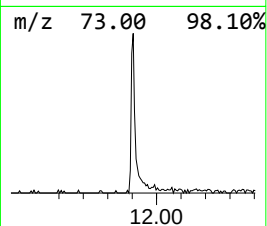
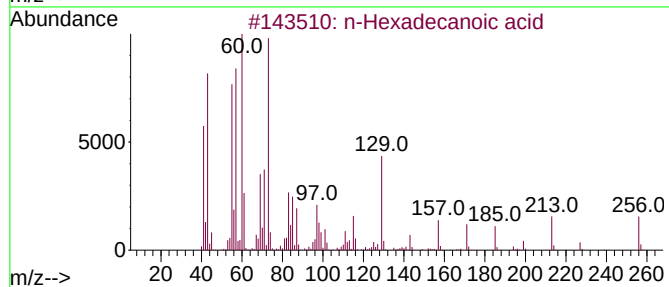
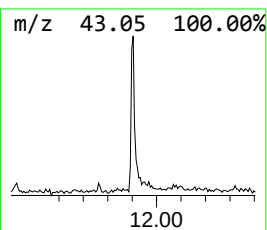
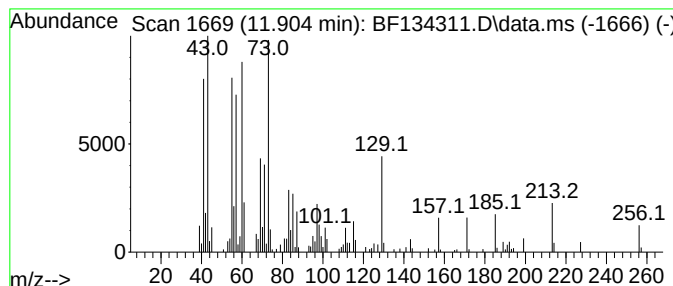
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.74 ng	161547	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Undecanoic acid	186	C11H22O2	000112-37-8	62
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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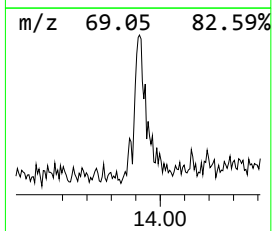
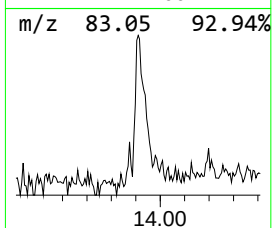
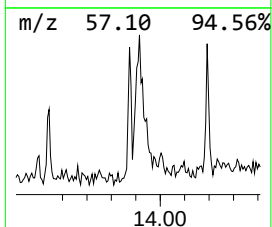
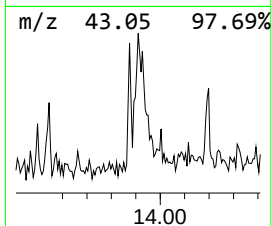
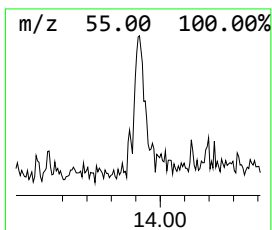
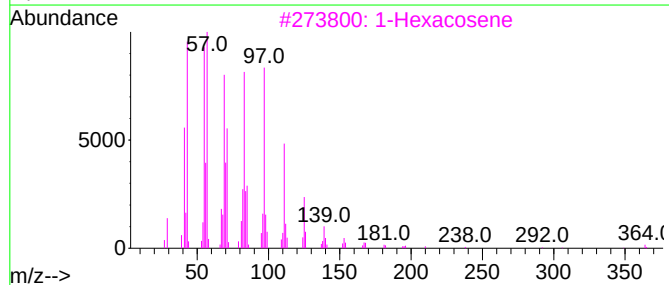
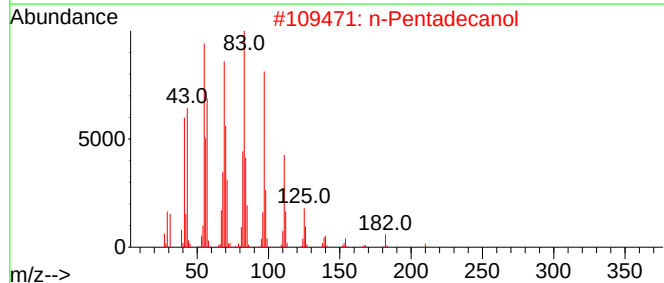
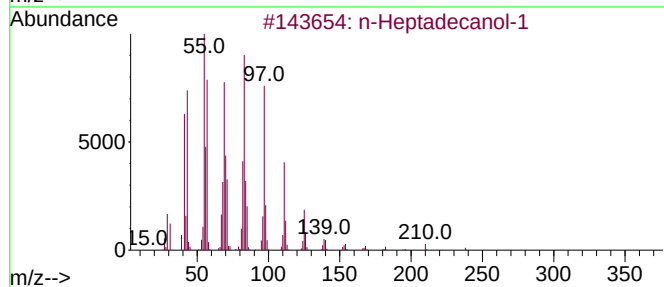
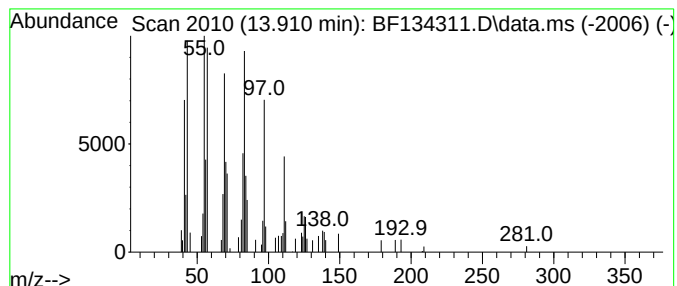
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Heptadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	2.63 ng	77046	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Heptadecanol-1	256	C17H36O	001454-85-9	94
2		n-Pentadecanol	228	C15H32O	000629-76-5	91
3		1-Hexacosene	364	C26H52	018835-33-1	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		1-Tricosene	322	C23H46	018835-32-0	91



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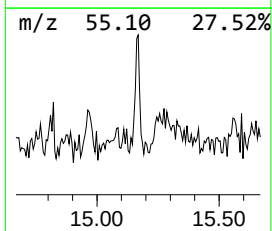
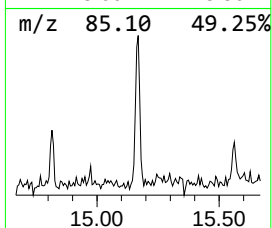
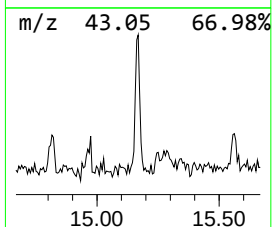
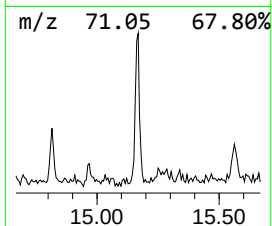
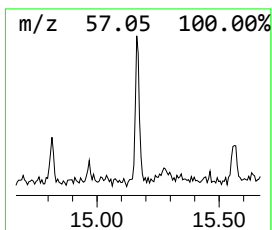
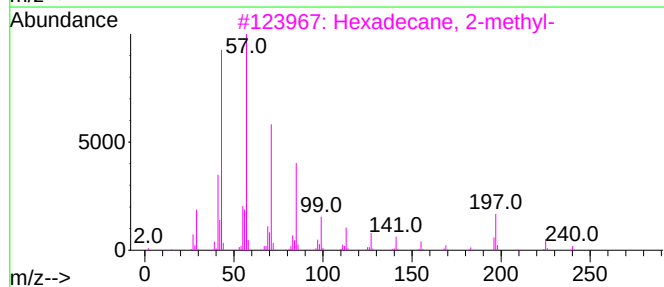
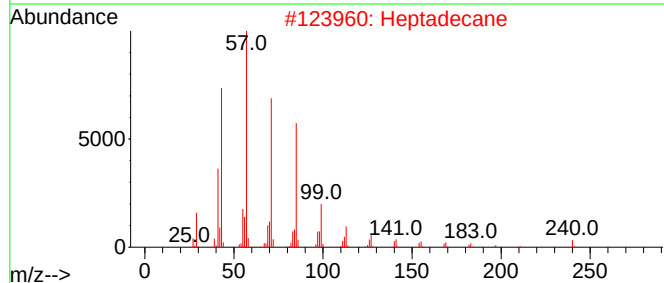
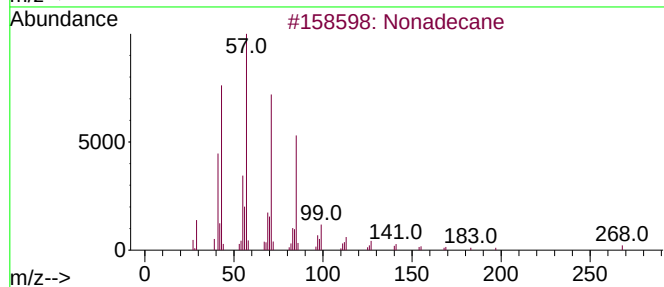
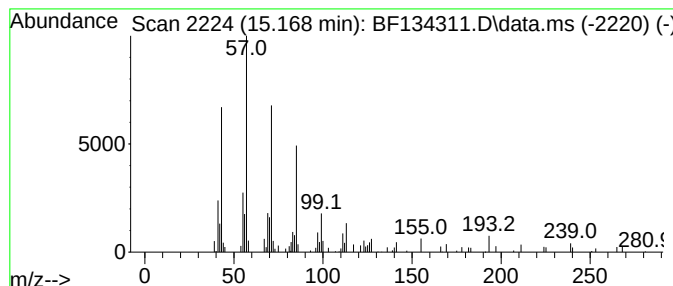
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	2.45 ng	52994	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	98
2			Heptadecane	240	C17H36	000629-78-7	93
3			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	93
4			Hexacosane	366	C26H54	000630-01-3	90
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	89



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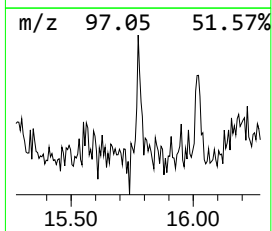
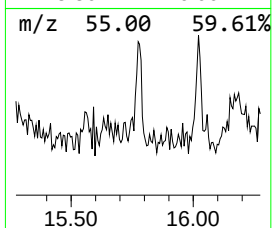
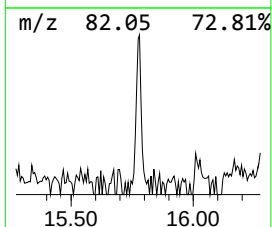
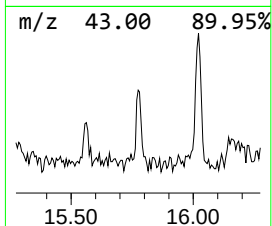
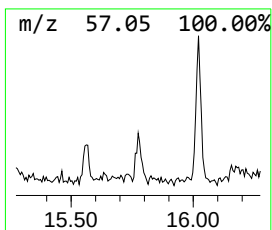
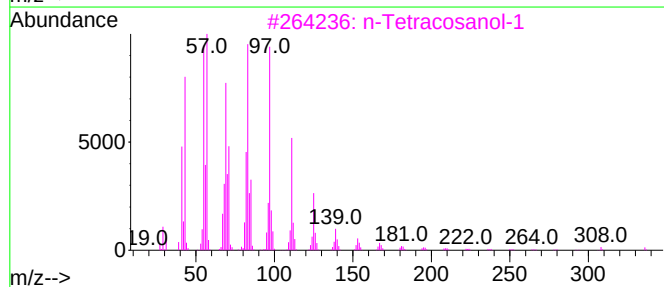
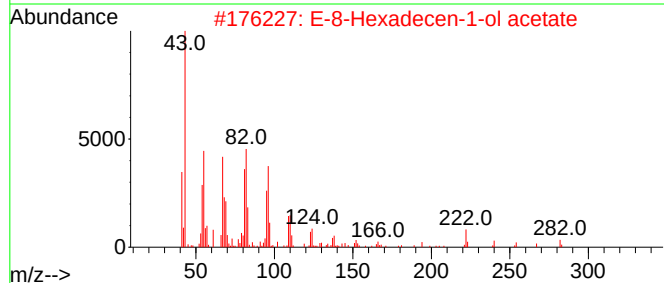
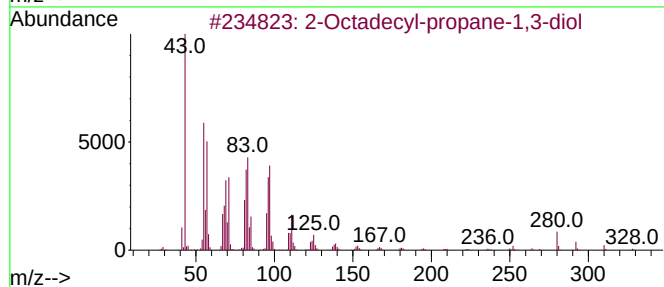
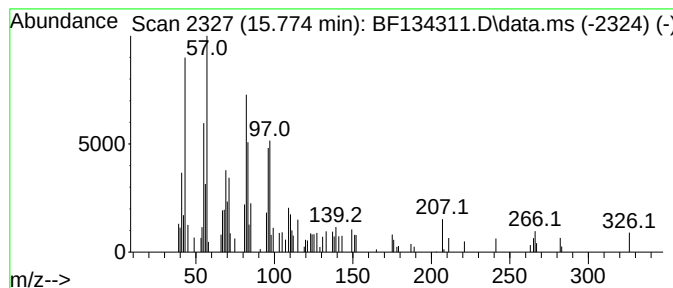
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Octadecyl-propane-1,3-diol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	2.08 ng	44934	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	58
2			E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	45
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	43
4			1-Eicosanol	298	C20H42O	000629-96-9	38
5			7-Azabicyclo[4.1.0]heptane, 1-me...	111	C7H13N	025022-25-7	38



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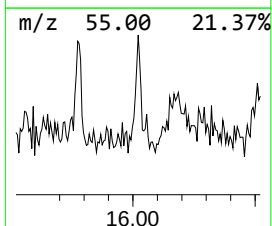
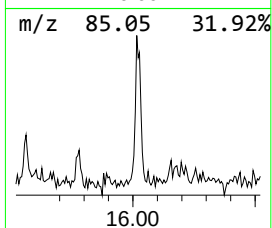
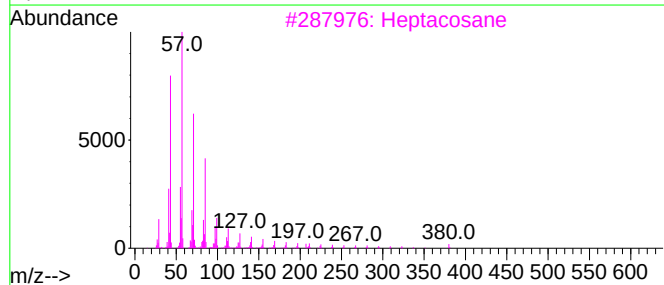
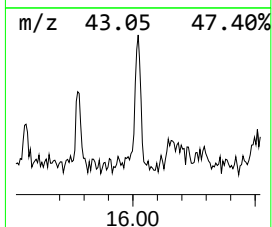
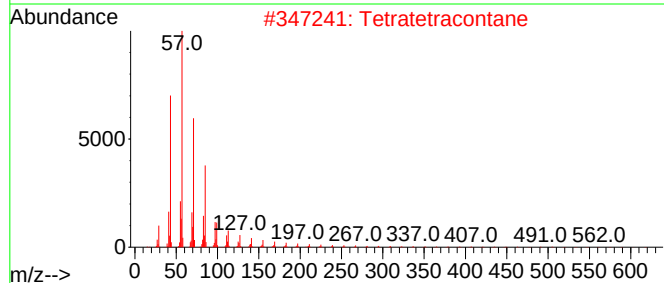
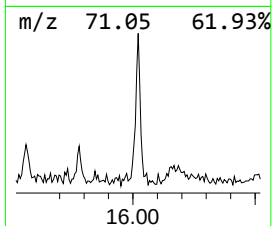
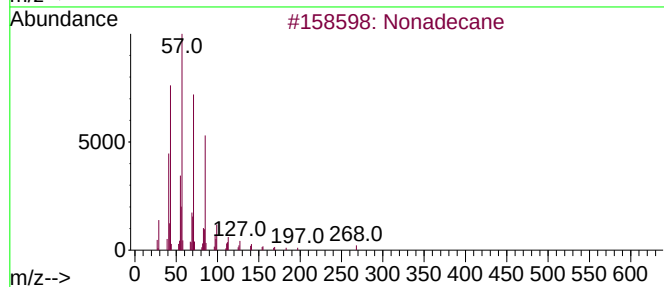
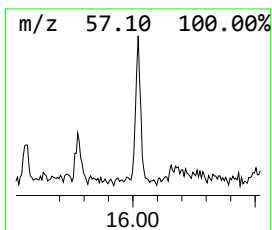
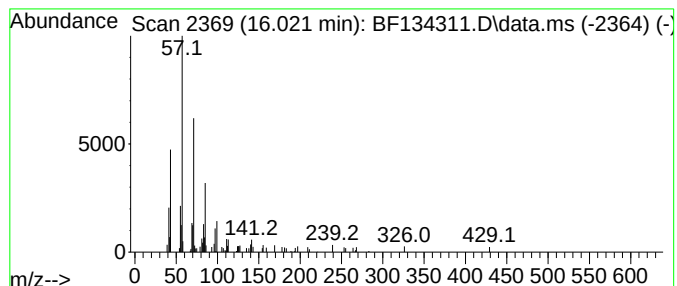
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 7 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.021	2.77 ng	59796	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Tetratetracontane	619	C44H90	007098-22-8	83
3			Heptacosane	380	C27H56	000593-49-7	80
4			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80
5			Hentriacontane	437	C31H64	000630-04-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134311.D
Acq On : 15 Jul 2023 03:09
Operator : CG\JU
Sample : 03597-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-46-(0-2)

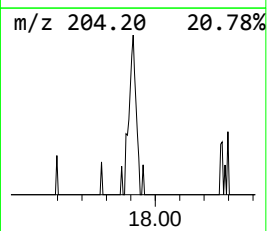
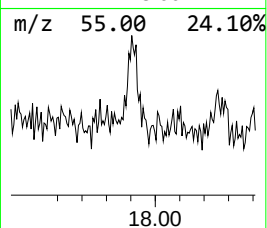
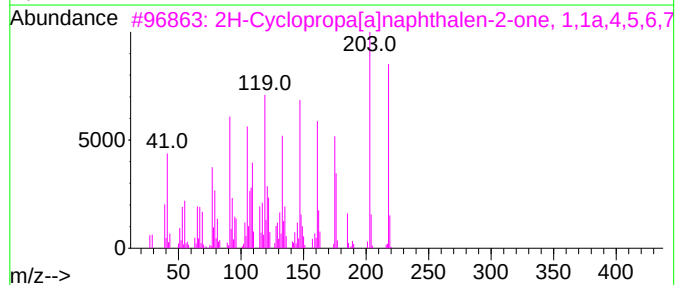
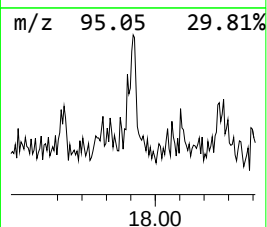
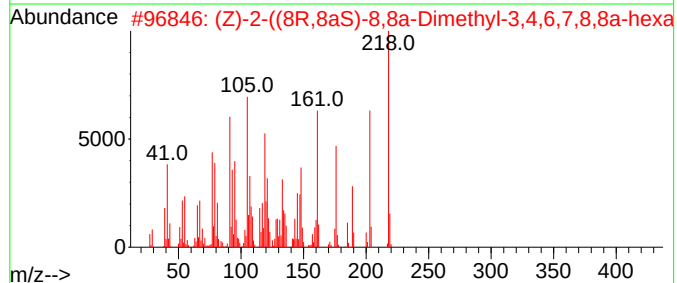
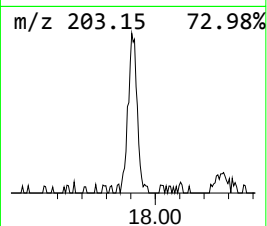
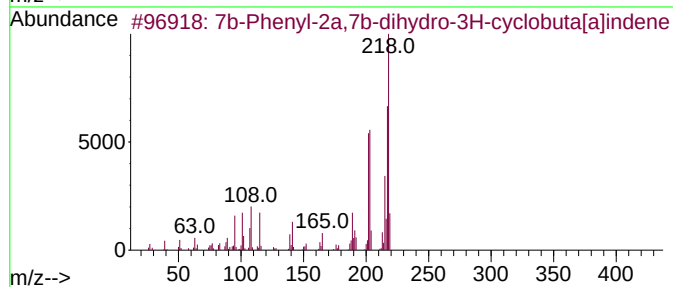
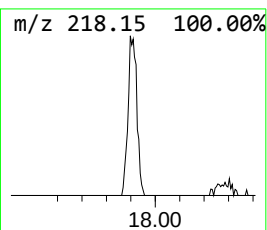
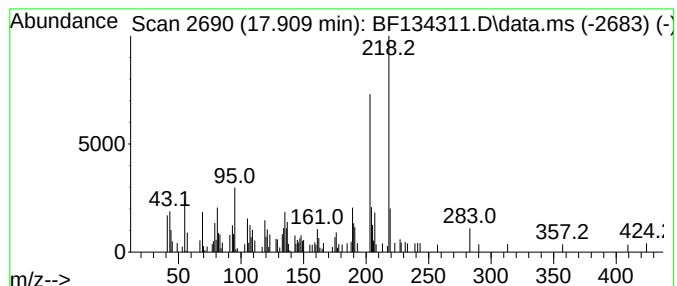
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 7b-Phenyl-2a,7b-dihydro-3H-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.909	5.52 ng	119315	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	72
2		(Z)-2-((8R,8aS)-8,8a-Dimethyl-3,...	218	C15H22O	137695-20-6	68
3		2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	58
4		Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	50
5		Pyrene, hexadecahydro-	218	C16H26	002435-85-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134311.D
Acq On : 15 Jul 2023 03:09
Operator : CG\JU
Sample : 03597-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-46-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.904	4.7	ng	161547	4	11.374	681456	20.0
n-Heptadecanol-1	13.910	2.6	ng	77046	5	14.033	585051	20.0
Nonadecane	15.168	2.5	ng	52994	6	15.539	432331	20.0
2-Octadecyl-pro...	15.774	2.1	ng	44934	6	15.539	432331	20.0
Tetratetracontane	16.021	2.8	ng	59796	6	15.539	432331	20.0
7b-Phenyl-2a,7b...	17.909	5.5	ng	119315	6	15.539	432331	20.0