

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
 Data File : BF135413.D
 Acq On : 22 Sep 2023 22:19
 Operator : CG\JU
 Sample : 04491-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B102-04

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.392	558	562	585	rBV	3237108	3243601	100.00%	13.435%
2	5.598	594	597	604	rBV2	53395	66691	2.06%	0.276%
3	6.404	730	734	744	rBV	3198526	3138918	96.77%	13.001%
4	6.592	761	766	771	rBV2	69618	94400	2.91%	0.391%
5	6.633	771	773	780	rVB3	36928	42978	1.33%	0.178%
6	6.757	791	794	801	rVB	1251869	997468	30.75%	4.131%
7	7.016	835	838	844	rVB	32835	39853	1.23%	0.165%
8	7.322	886	890	893	rBV	2283884	1997122	61.57%	8.272%
9	7.610	937	939	952	rVB	99078	113252	3.49%	0.469%
10	7.839	975	978	984	rVB3	25873	34182	1.05%	0.142%
11	8.033	1005	1011	1015	rBV	1405908	1241394	38.27%	5.142%
12	8.251	1043	1048	1052	rBV	71057	69973	2.16%	0.290%
13	8.310	1056	1058	1066	rVB2	75118	82433	2.54%	0.341%
14	8.745	1129	1132	1136	rBV2	37611	40705	1.25%	0.169%
15	9.116	1188	1195	1198	rBV	3024094	2839706	87.55%	11.762%
16	9.239	1210	1216	1219	rBV3	51699	87169	2.69%	0.361%
17	9.651	1284	1286	1291	rBV	33919	42876	1.32%	0.178%
18	9.792	1306	1310	1321	rVB	1426672	1219308	37.59%	5.050%
19	10.327	1398	1401	1410	rVB4	35122	54380	1.68%	0.225%
20	10.586	1441	1445	1453	rBV	1538365	1471928	45.38%	6.097%
21	10.651	1453	1456	1463	rVV3	58799	101443	3.13%	0.420%
22	10.710	1463	1466	1471	rVB7	19770	32901	1.01%	0.136%
23	11.286	1560	1564	1566	rBV	1063051	979776	30.21%	4.058%
24	11.310	1566	1568	1571	rVB	89077	74822	2.31%	0.310%
25	11.821	1652	1655	1659	rBV	347428	358398	11.05%	1.484%
26	12.504	1768	1771	1774	rBV	168386	141102	4.35%	0.584%
27	12.610	1786	1789	1794	rBV5	86037	98467	3.04%	0.408%
28	12.733	1807	1810	1816	rVB	177260	148838	4.59%	0.616%
29	12.880	1831	1835	1838	rBV	2088501	1756076	54.14%	7.273%
30	13.368	1914	1918	1927	rBV	775552	786859	24.26%	3.259%
31	13.792	1988	1990	1996	rVB3	58400	60922	1.88%	0.252%
32	13.857	1996	2001	2008	rBV6	74185	212840	6.56%	0.882%
33	13.939	2011	2015	2018	rVV	910133	978188	30.16%	4.052%
34	13.968	2018	2020	2025	rVB	93414	92953	2.87%	0.385%
35	14.468	2102	2105	2109	rBV	299932	316854	9.77%	1.312%
36	14.980	2190	2192	2196	rBV	88332	106704	3.29%	0.442%

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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_F\Methods\8270-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.409	2261	2265	2278	rVB	731428	978065	30.15%	4.051%
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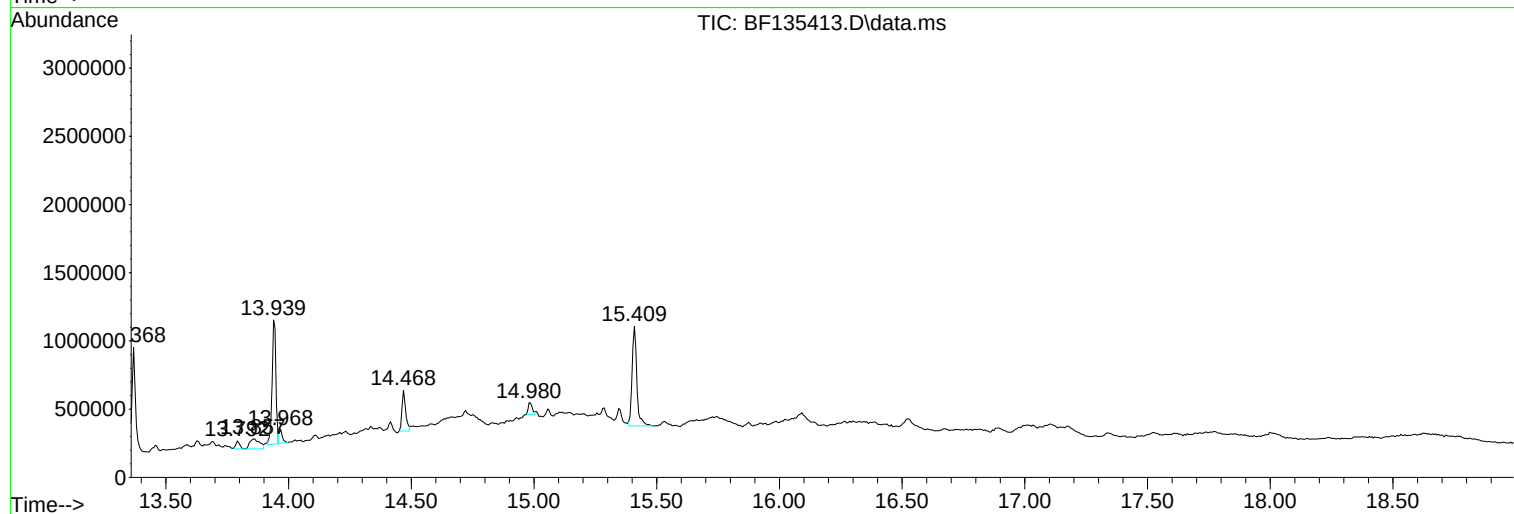
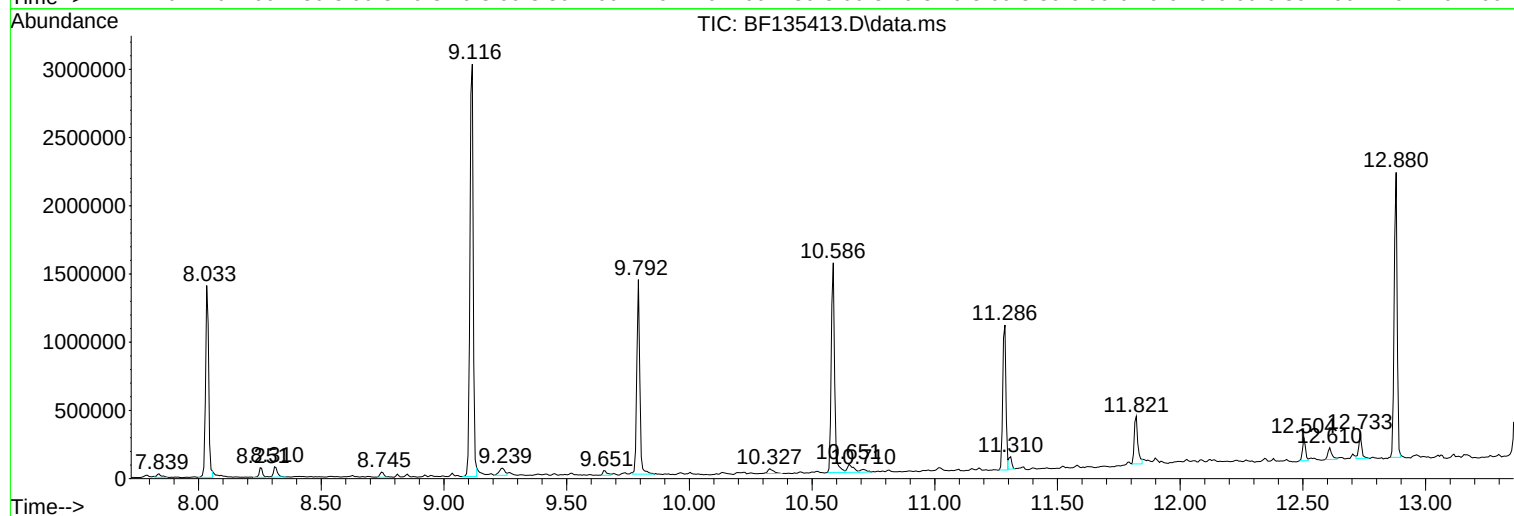
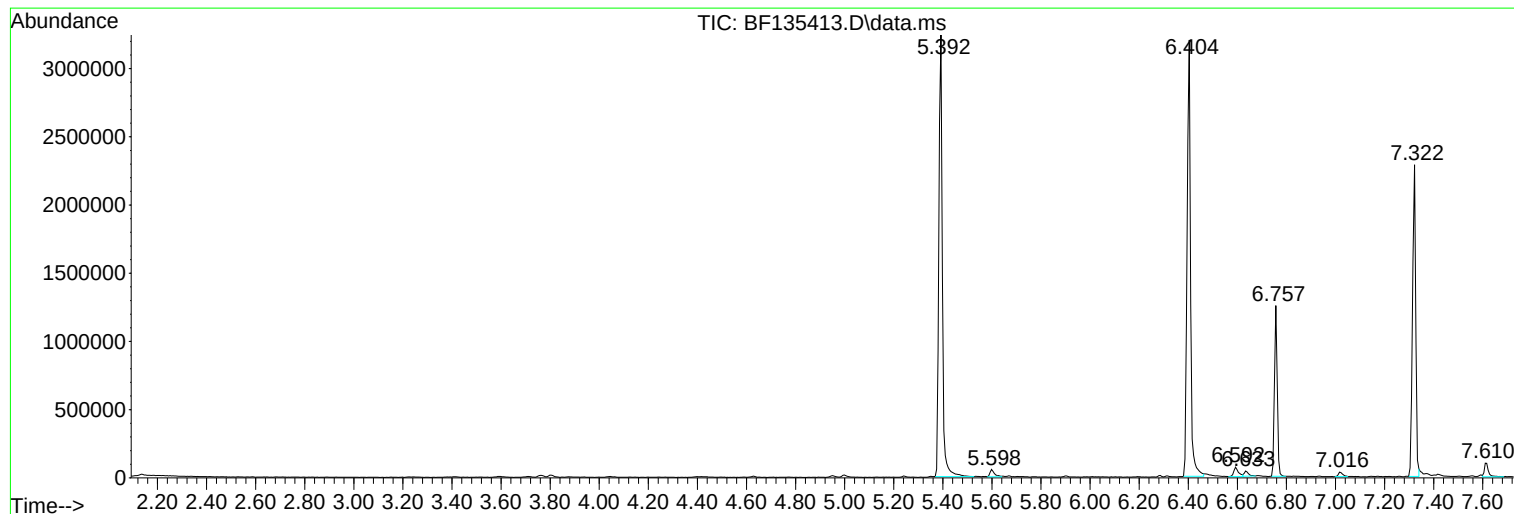
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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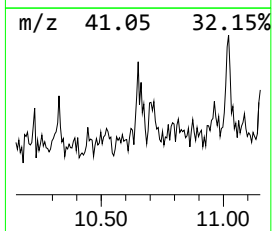
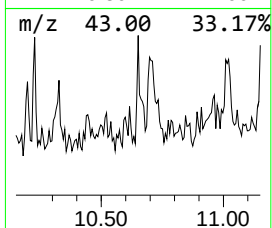
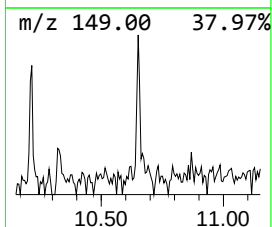
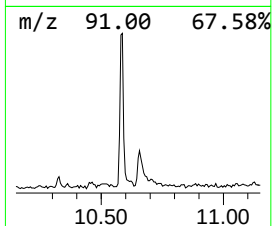
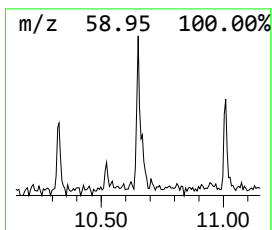
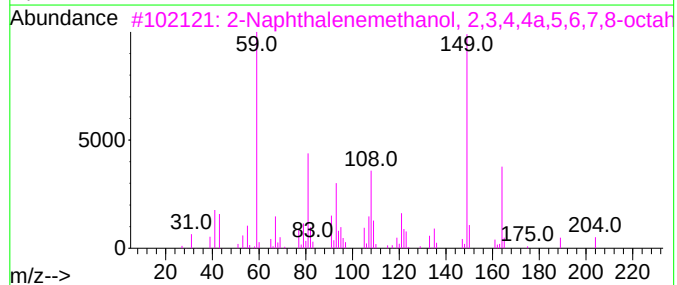
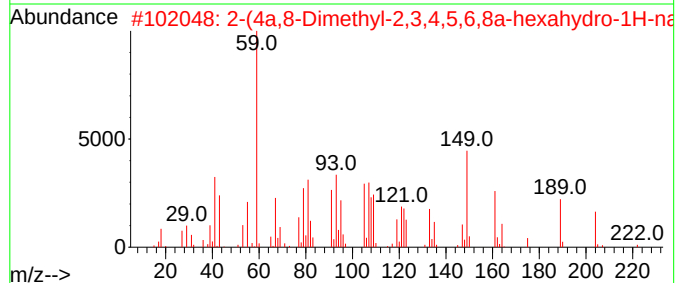
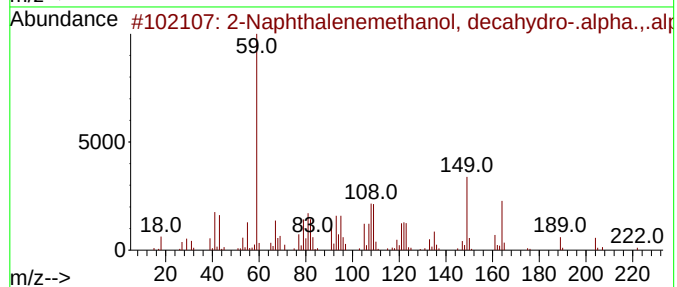
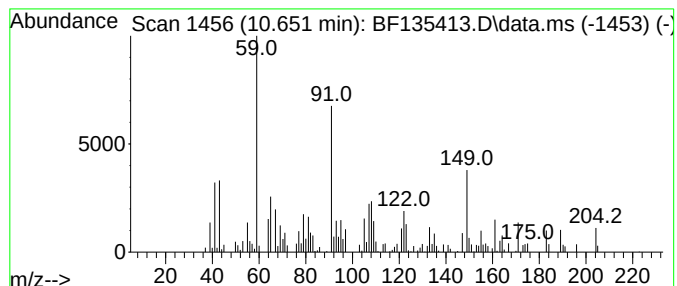
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Naphthalenemethanol, deca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.07 ng	101443	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenemethanol, decahydro...	222	C15H26O	000473-15-4	59		
2	2-(4a,8-Dimethyl-2,3,4,5,6,8a-he...	222	C15H26O	1000411-50-1	50		
3	2-Naphthalenemethanol, 2,3,4,4a,...	222	C15H26O	063891-61-2	40		
4	2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	079254-46-9	38		
5	2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	000473-16-5	35		



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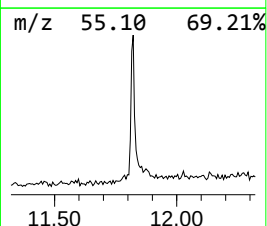
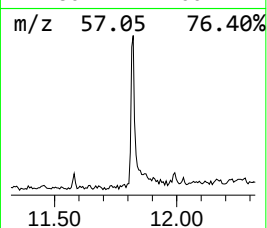
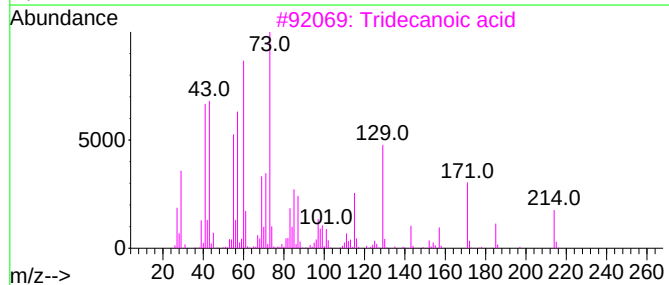
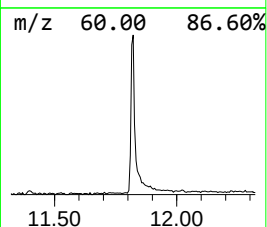
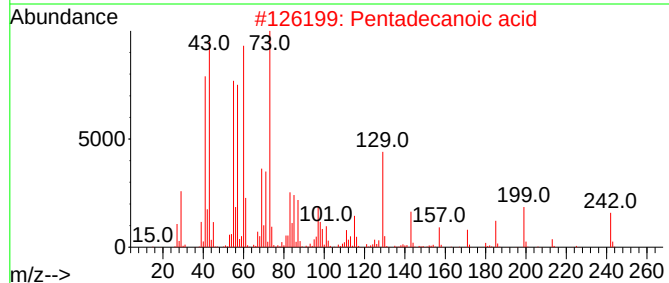
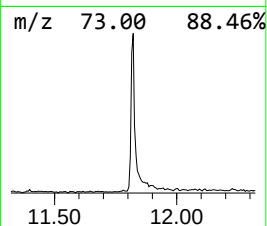
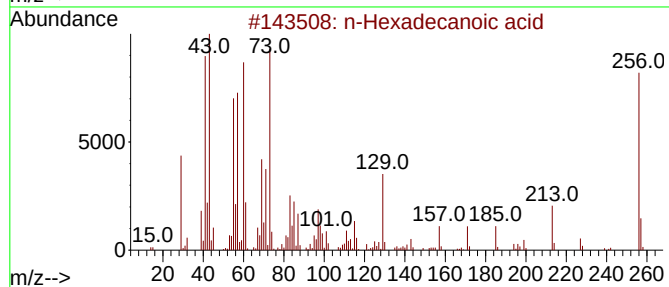
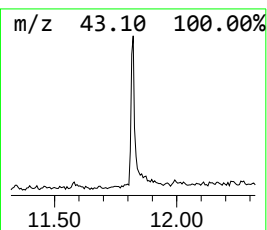
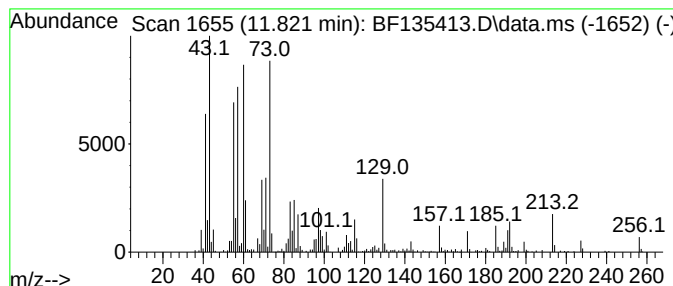
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	7.32 ng	358398	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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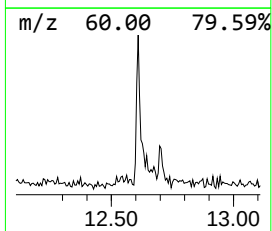
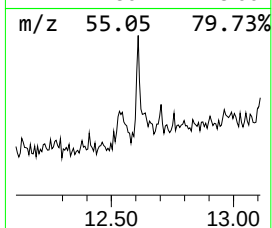
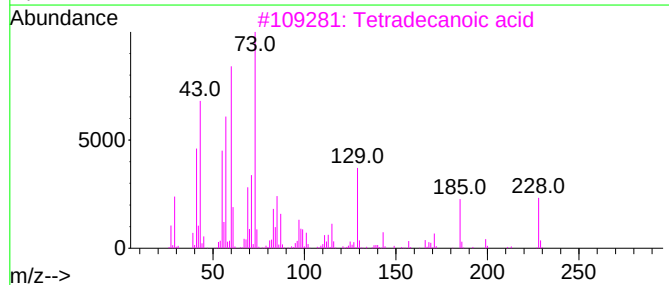
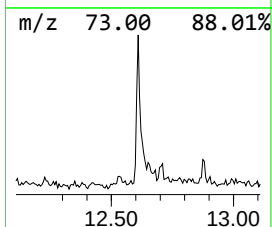
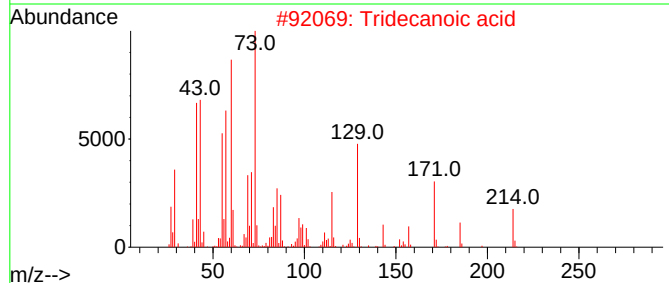
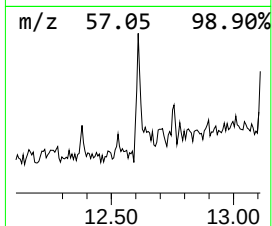
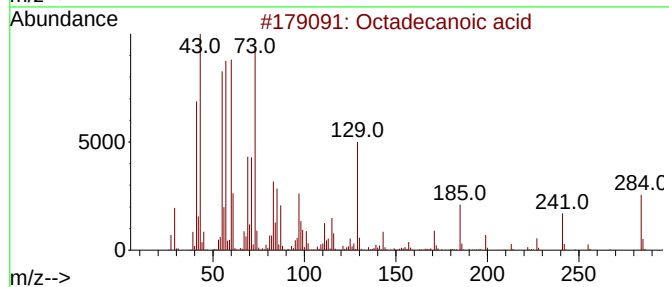
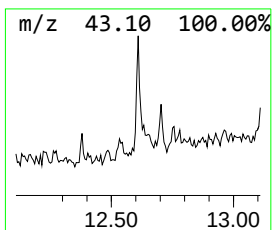
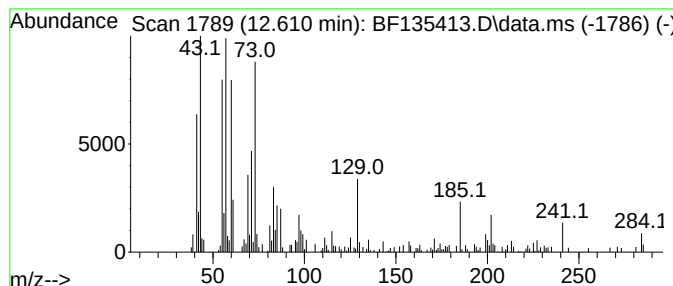
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	2.01 ng	98467	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Dodecanoic acid	200	C12H24O2	000143-07-7	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



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ALS Vial : 14 Sample Multiplier: 1

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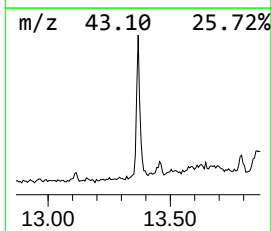
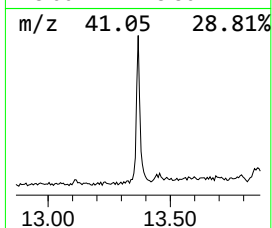
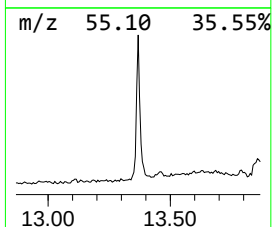
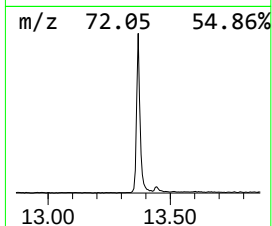
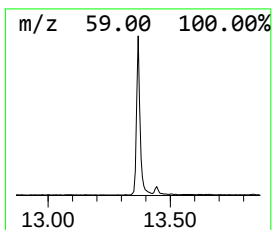
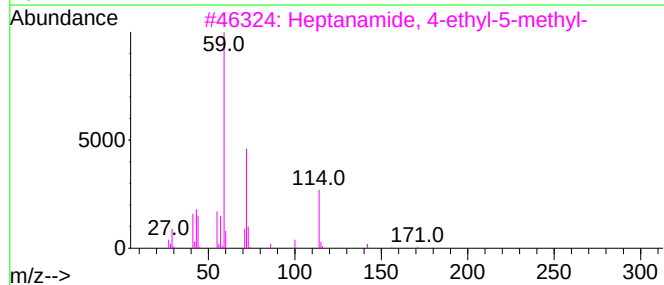
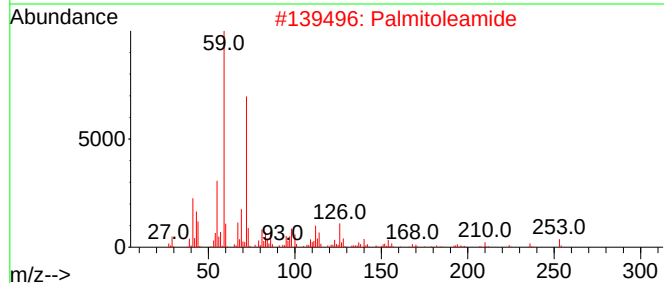
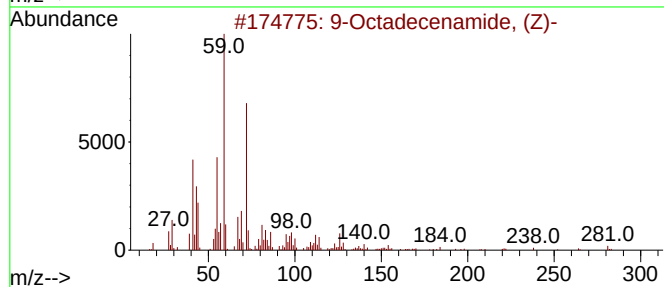
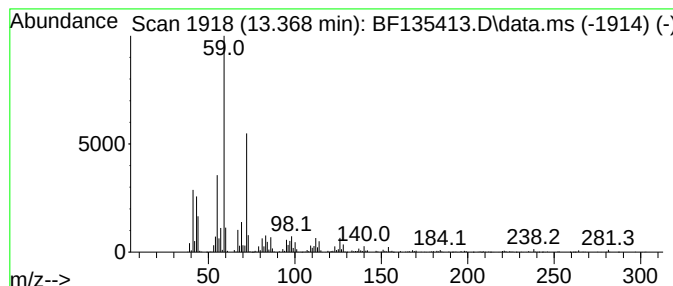
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	16.09 ng	786859	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2			Palmitoleamide	253	C16H31NO	106010-22-4	58
3			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
4			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5			Methyl 2-[(2-methoxypropanoyl)(m...	231	C11H21NO4	1000495-86-7	47



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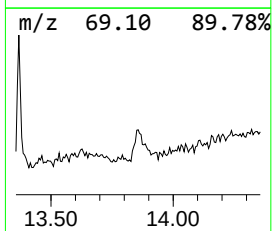
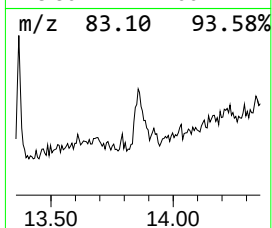
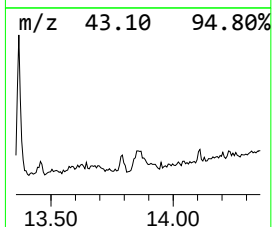
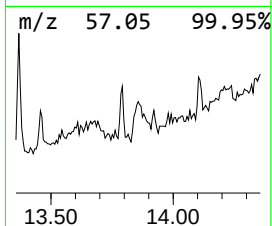
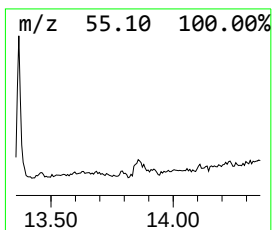
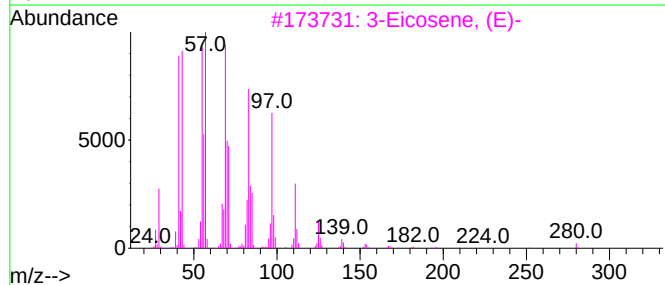
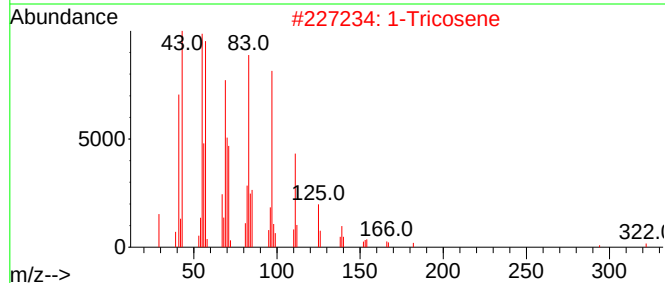
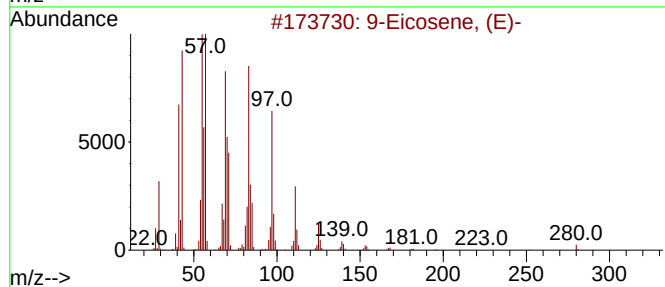
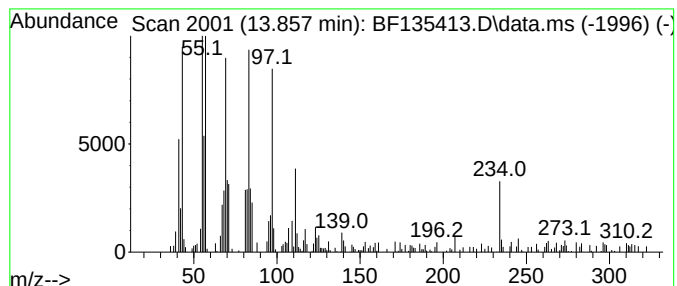
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	4.35 ng	212840	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Eicosene, (E)-	280	C20H40	074685-29-3	93
2		1-Tricosene	322	C23H46	018835-32-0	93
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4		9-Tricosene, (Z)-	322	C23H46	027519-02-4	83
5		Cycloeicosane	280	C20H40	000296-56-0	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135413.D
Acq On : 22 Sep 2023 22:19
Operator : CG\JU
Sample : 04491-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B102-04

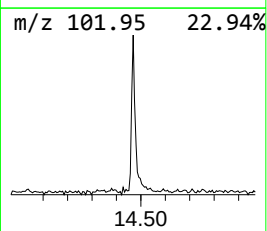
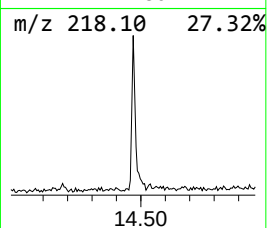
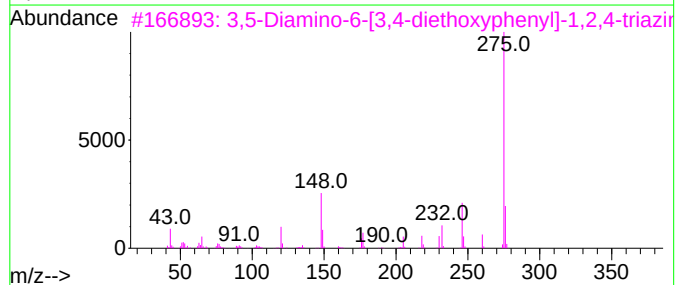
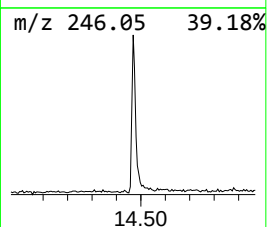
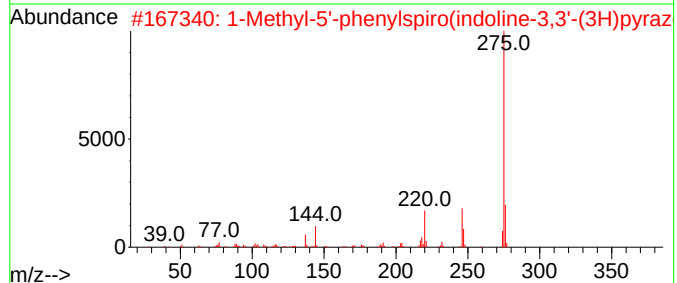
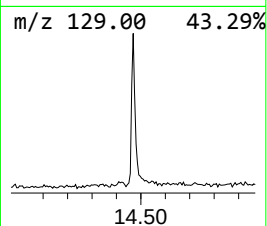
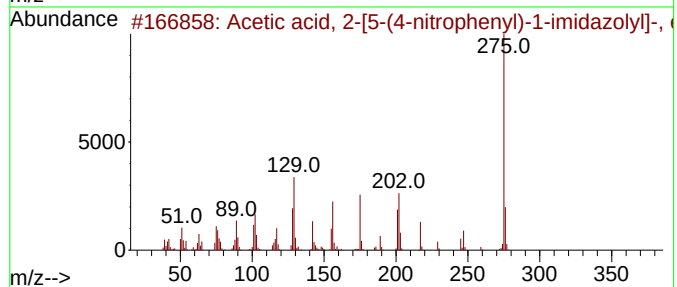
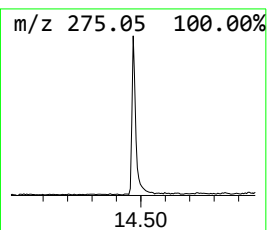
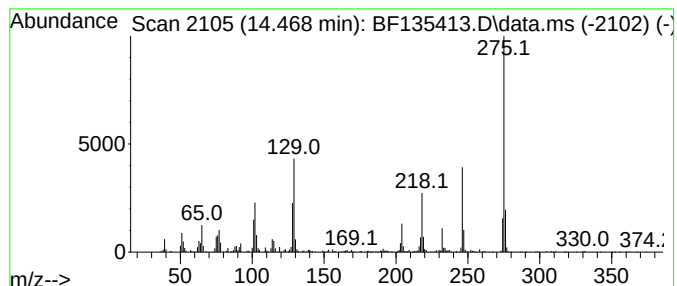
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.468 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.468	6.48 ng	316854	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-[5-(4-nitrophenyl)...	275	C13H13N3O4	351064-45-4	49
2			1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	43
3			3,5-Diamino-6-[3,4-diethoxypheny...	275	C13H17N5O2	058848-69-4	37
4			5H-[1]Benzopyrano[4,3-d]pyrimidi...	275	C16H9N3O2	1000337-49-1	27
5			1H-Pyrazolo[4',3':5,6]pyrido[2,3...	275	C12H13N5O3	349496-02-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
Data File : BF135413.D
Acq On : 22 Sep 2023 22:19
Operator : CG\JU
Sample : 04491-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B102-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
2-Naphthaleneme...	10.651	2.1	ng	101443	4	11.286	979776	20.0
n-Hexadecanoic ...	11.821	7.3	ng	358398	4	11.286	979776	20.0
Octadecanoic acid	12.610	2.0	ng	98467	4	11.286	979776	20.0
9-Octadecenamid...	13.368	16.1	ng	786859	5	13.939	978188	20.0
9-Eicosene, (E)-	13.857	4.3	ng	212840	5	13.939	978188	20.0
unknown14.468	14.468	6.5	ng	316854	5	13.939	978188	20.0