

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
 Data File : BF136429.D
 Acq On : 06 Dec 2023 15:37
 Operator : CG\JU
 Sample : 05538-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-02-112223

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136429.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	497	500	505	rVB	21404	24624	1.42%	0.192%
2	5.428	564	568	571	rBV	1866464	1596190	92.33%	12.439%
3	6.428	734	738	741	rBV	1669548	1557796	90.11%	12.140%
4	6.792	797	800	804	rBV	636045	566035	32.74%	4.411%
5	7.357	891	896	899	rBV	1062409	974485	56.37%	7.594%
6	7.387	899	901	905	rVB2	25674	26091	1.51%	0.203%
7	7.434	905	909	913	rBV4	18275	23305	1.35%	0.182%
8	8.075	1012	1018	1021	rBV	794906	715448	41.39%	5.575%
9	8.363	1063	1067	1070	rBV6	15831	24440	1.41%	0.190%
10	8.498	1086	1090	1092	rBV	36237	34797	2.01%	0.271%
11	8.616	1106	1110	1113	rBV2	23093	23847	1.38%	0.186%
12	8.669	1115	1119	1122	rBV2	33837	31091	1.80%	0.242%
13	9.098	1189	1192	1197	rVB	45452	37368	2.16%	0.291%
14	9.151	1197	1201	1204	rBV	2295880	1728728	100.00%	13.472%
15	9.234	1210	1215	1218	rBV	53897	56609	3.27%	0.441%
16	9.269	1218	1221	1231	rVB2	74290	101066	5.85%	0.788%
17	9.533	1264	1266	1268	rBV2	21285	22466	1.30%	0.175%
18	9.551	1268	1269	1272	rVB	36677	28453	1.65%	0.222%
19	9.828	1309	1316	1320	rBV	754190	626576	36.24%	4.883%
20	10.616	1446	1450	1459	rBV	869964	763931	44.19%	5.953%
21	10.751	1469	1473	1476	rBV	37194	49691	2.87%	0.387%
22	11.222	1550	1553	1557	rVB2	24319	24861	1.44%	0.194%
23	11.316	1566	1569	1572	rBV	584179	520746	30.12%	4.058%
24	11.669	1623	1629	1633	rBV9	11448	27864	1.61%	0.217%
25	11.722	1633	1638	1644	rVB	48980	58665	3.39%	0.457%
26	11.857	1657	1661	1665	rBV2	99195	109552	6.34%	0.854%
27	12.110	1701	1704	1707	rVB	45073	34620	2.00%	0.270%
28	12.410	1752	1755	1757	rBV	242614	202351	11.71%	1.577%
29	12.433	1757	1759	1766	rVB	145448	127324	7.37%	0.992%
30	12.645	1792	1795	1799	rBV4	27771	32832	1.90%	0.256%
31	12.763	1813	1815	1818	rVB	28979	25480	1.47%	0.199%
32	12.916	1837	1841	1844	rBV	1867308	1536041	88.85%	11.970%
33	13.151	1879	1881	1885	rBV5	18886	23007	1.33%	0.179%
34	13.969	2016	2020	2024	rBV	646891	591785	34.23%	4.612%
35	14.839	2165	2168	2171	rBV	71485	72963	4.22%	0.569%
36	15.451	2268	2272	2279	rVB	353916	431295	24.95%	3.361%

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ClientSampleId :
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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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

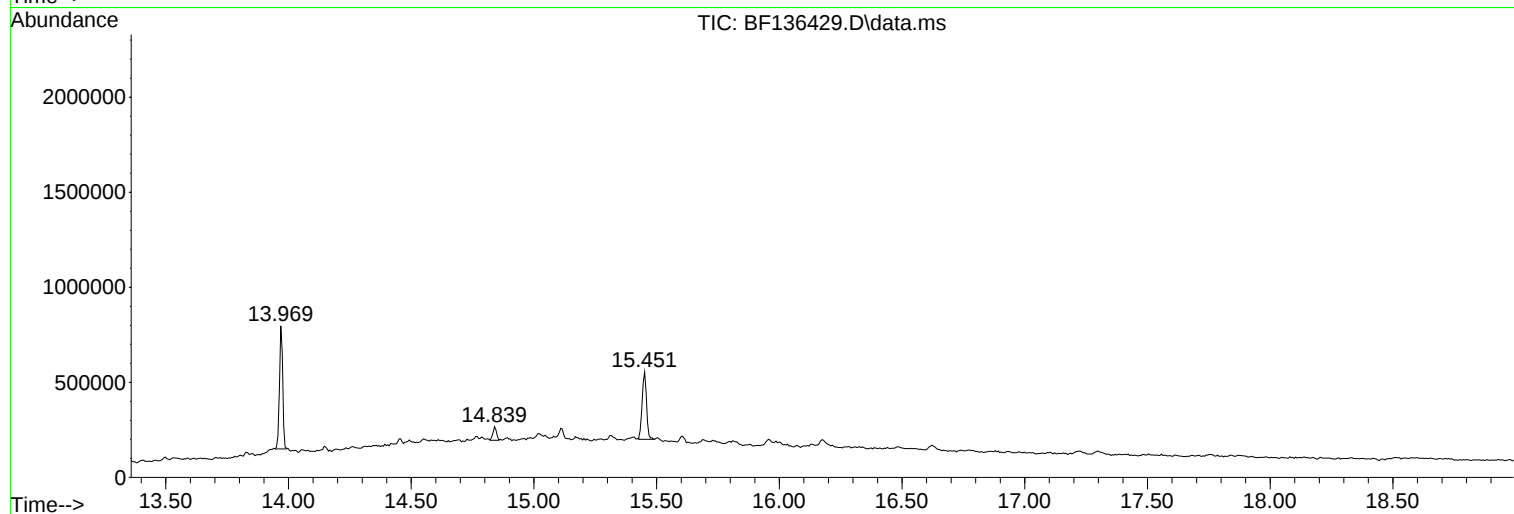
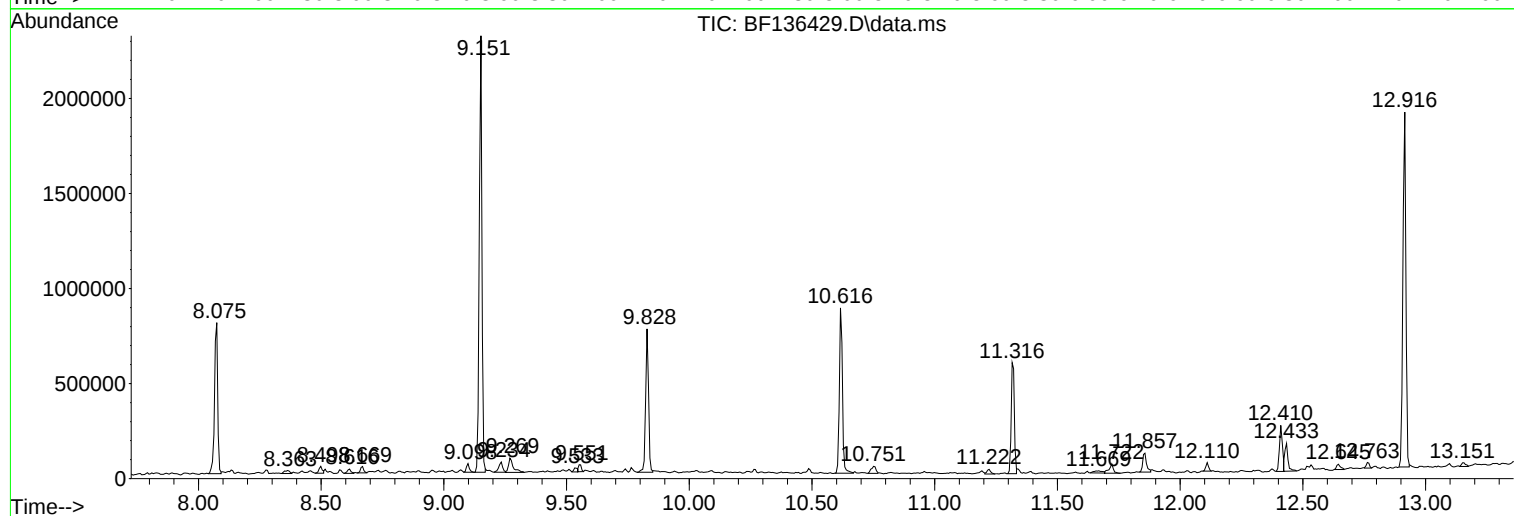
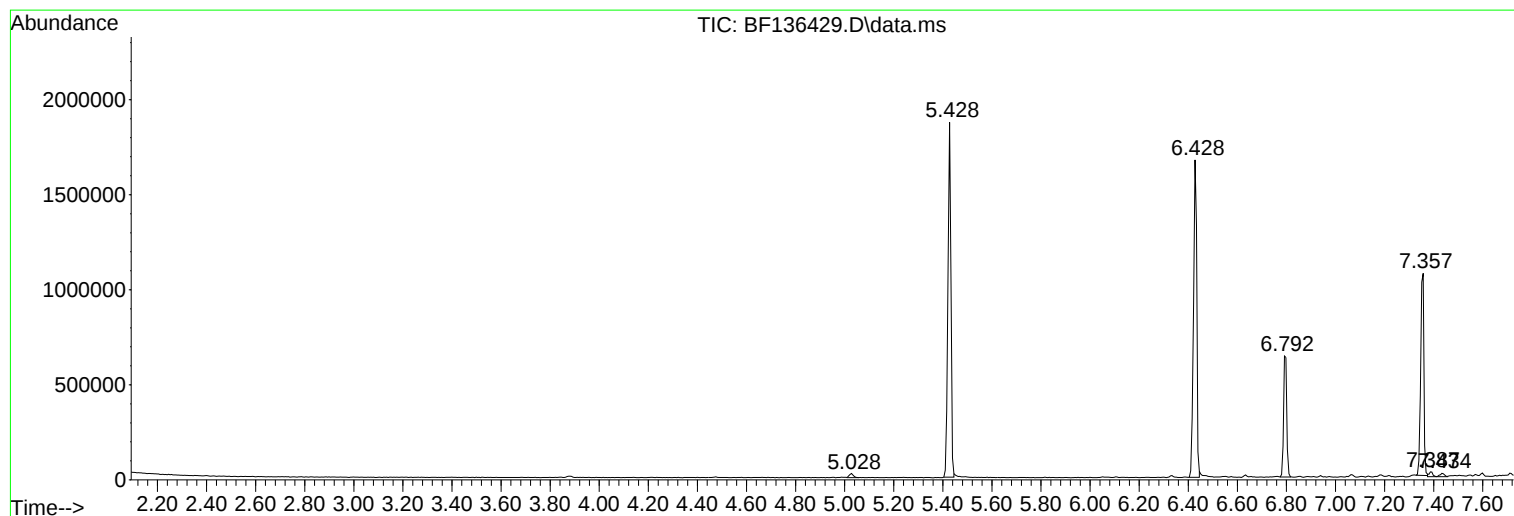
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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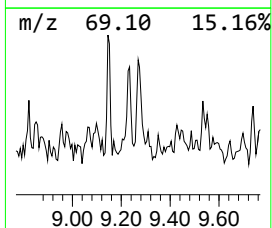
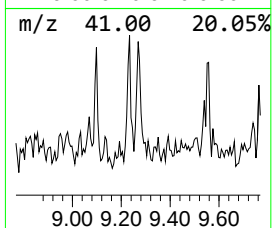
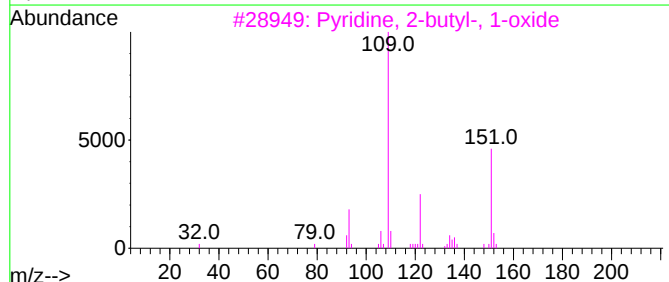
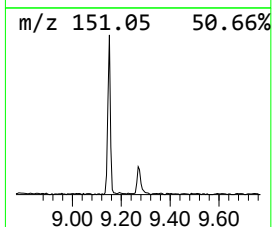
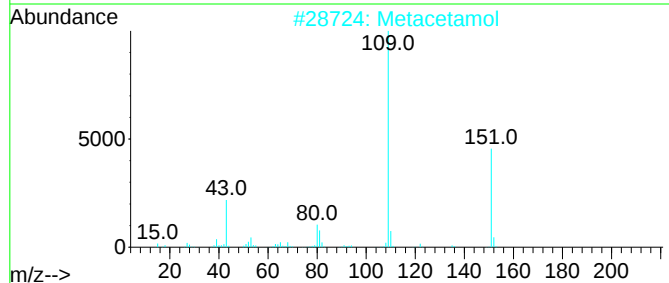
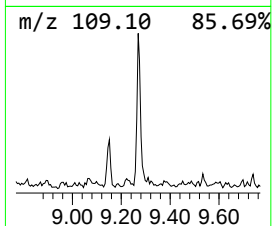
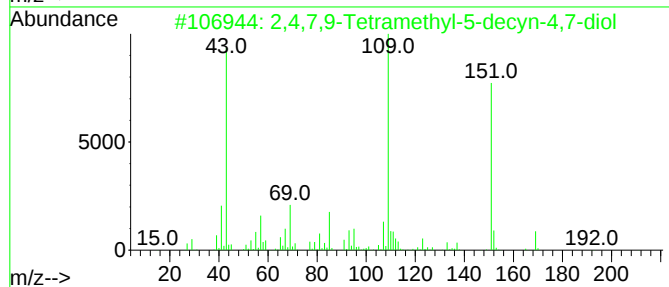
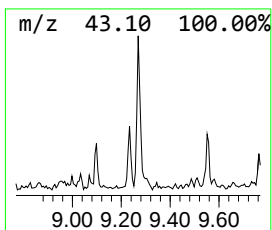
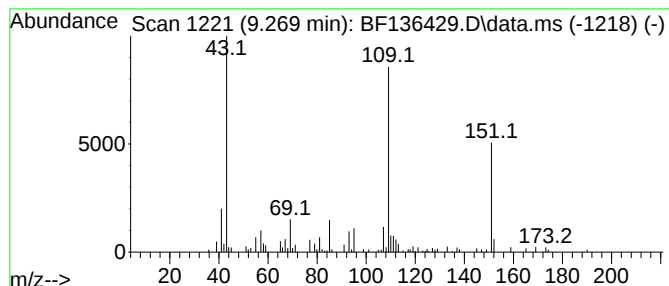
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	3.23 ng	101066	Acenaphthene-d10	9.828

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	59		
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59		
4	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	56		
5	6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	43		



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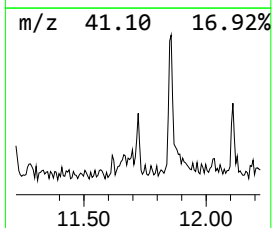
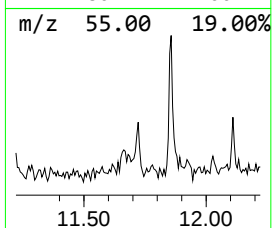
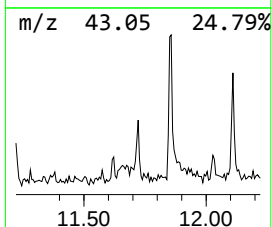
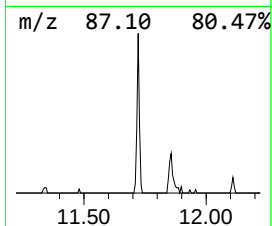
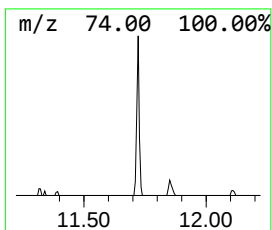
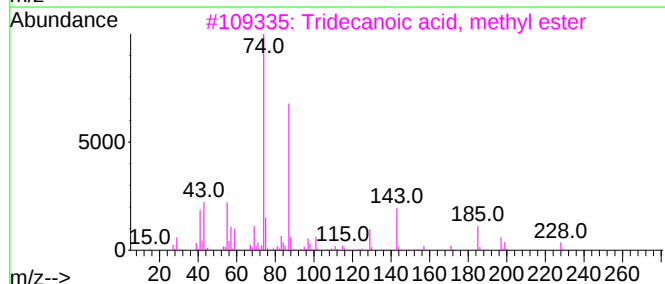
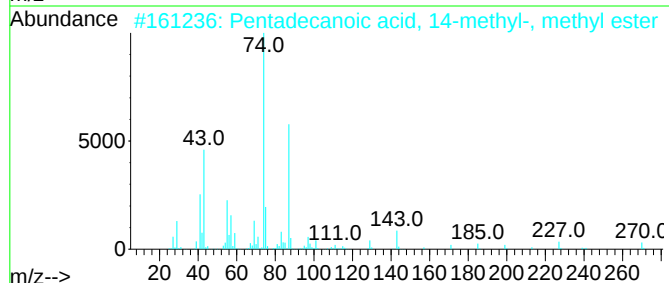
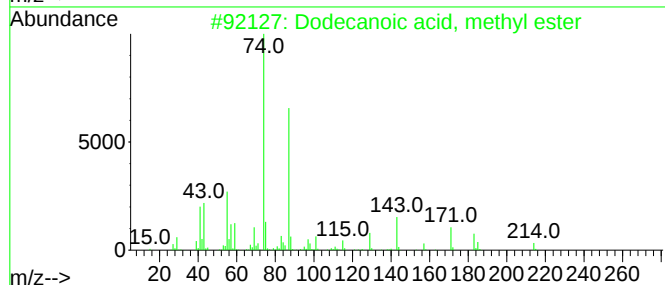
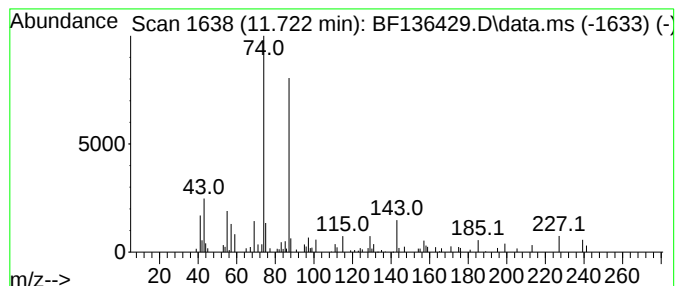
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Dodecanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.722	2.25 ng	58665	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	78
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	53
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	50
5			Undecanoic acid, 2-methyl-	200	C12H24O2	024323-25-9	50



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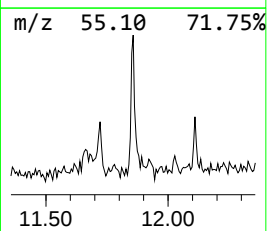
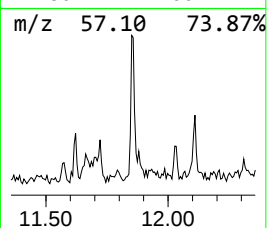
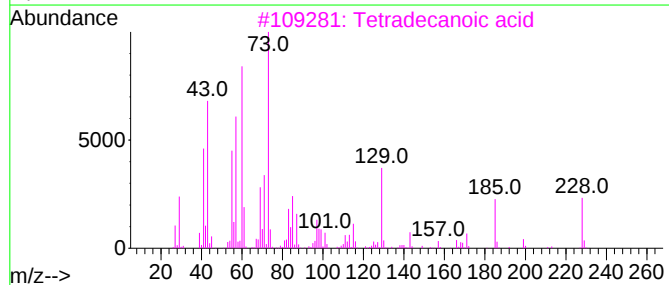
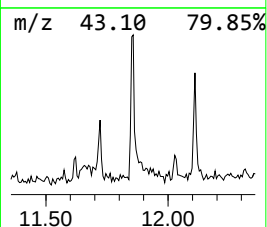
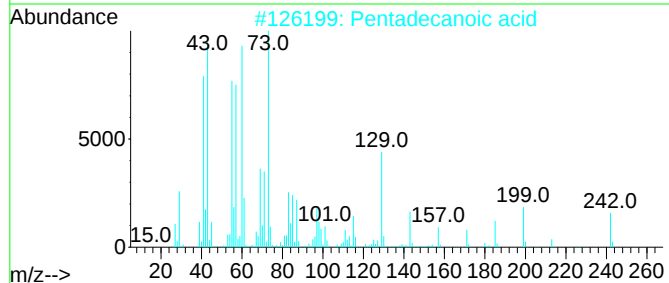
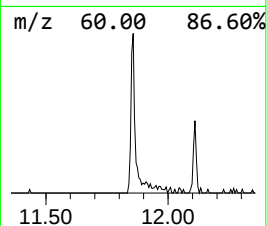
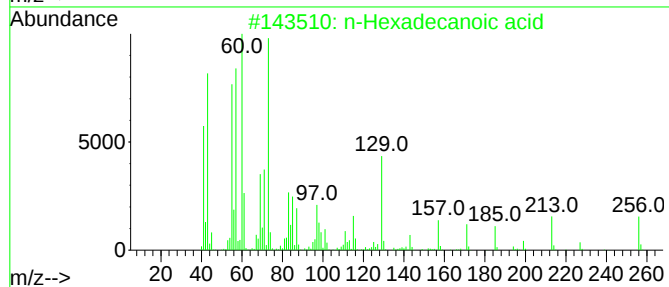
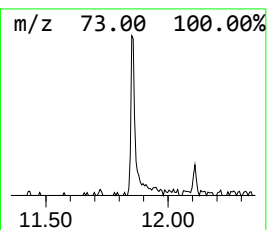
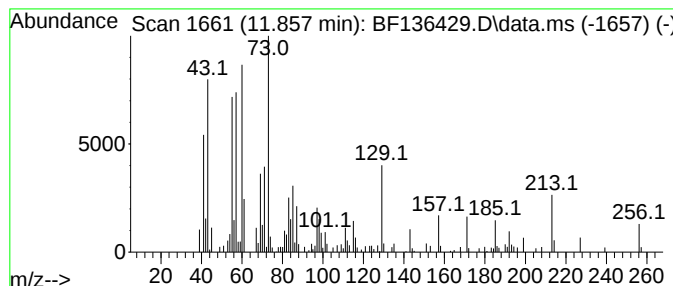
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.21 ng	109552	Phenanthrene-d10	11.316

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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ALS Vial : 12 Sample Multiplier: 1

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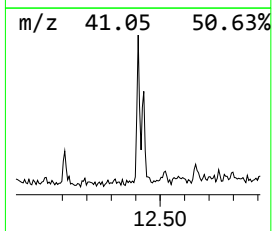
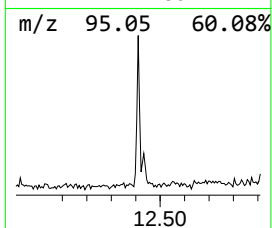
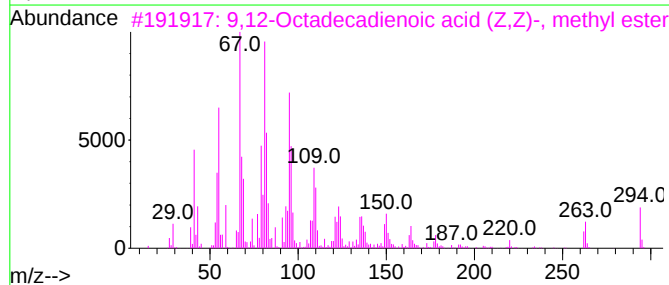
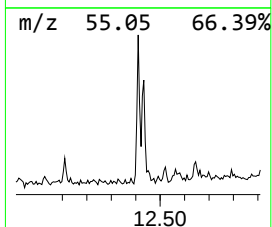
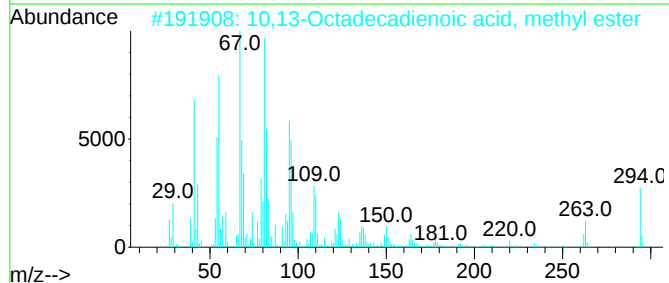
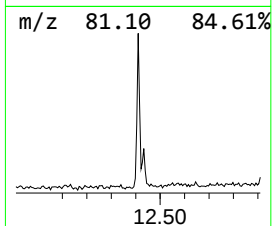
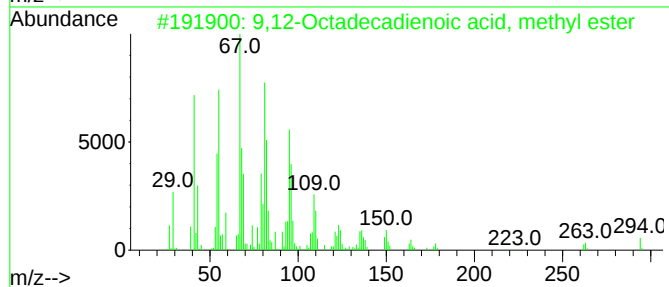
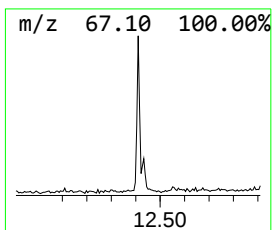
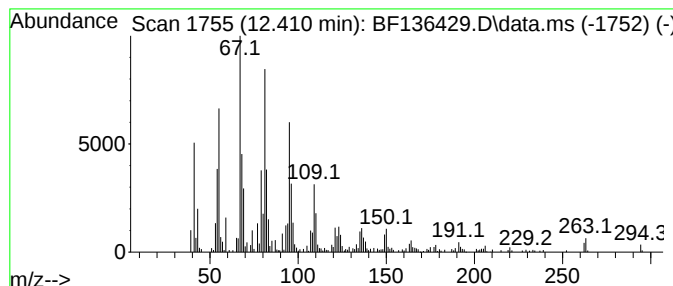
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	7.77 ng	202351	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98		
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98		
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98		
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98		



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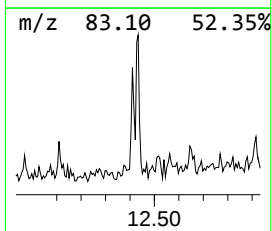
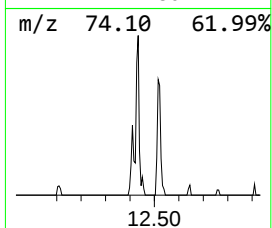
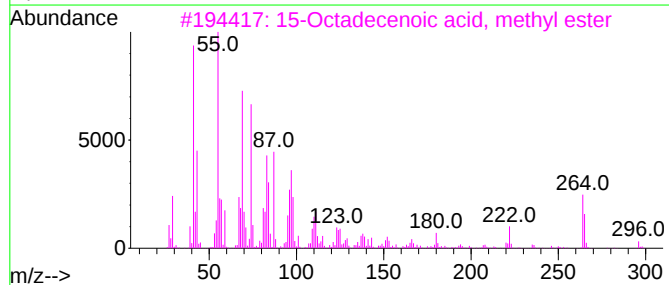
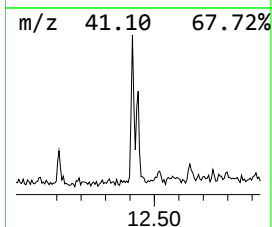
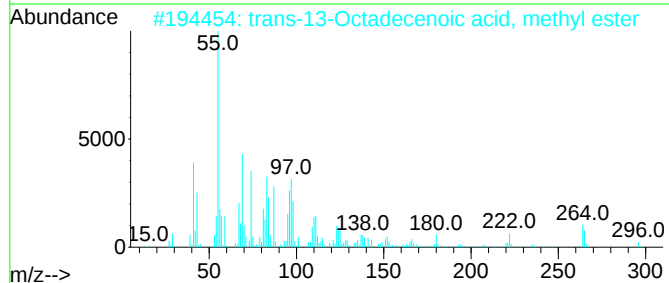
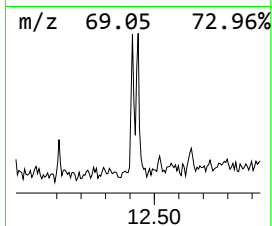
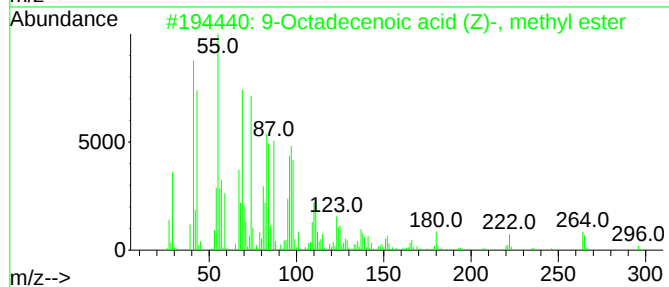
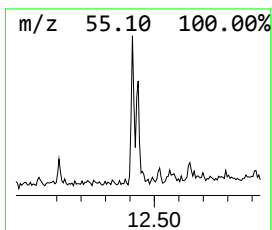
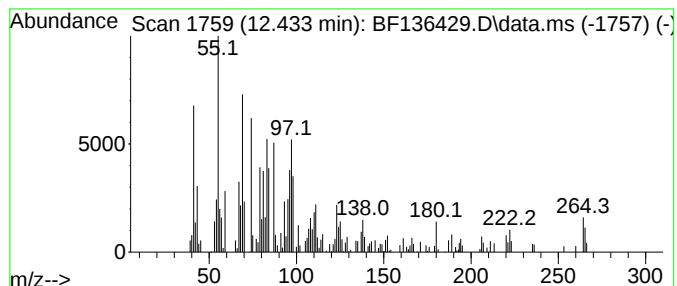
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.433	4.89 ng	127324	Phenanthrene-d10	11.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
4	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	90
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136429.D
Acq On : 06 Dec 2023 15:37
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-112223

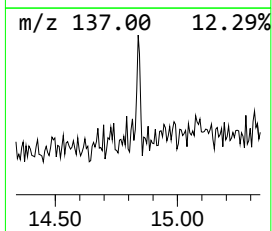
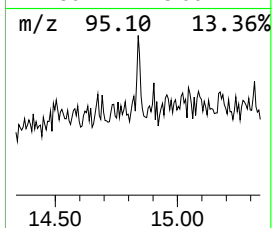
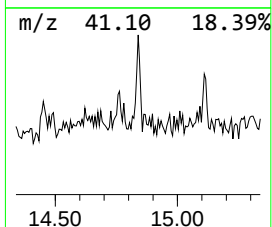
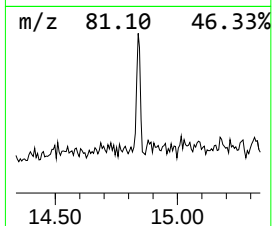
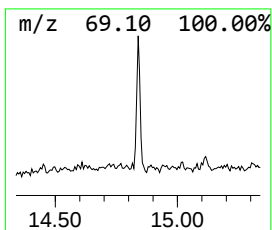
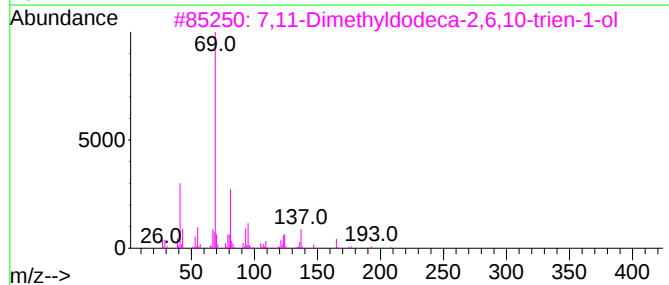
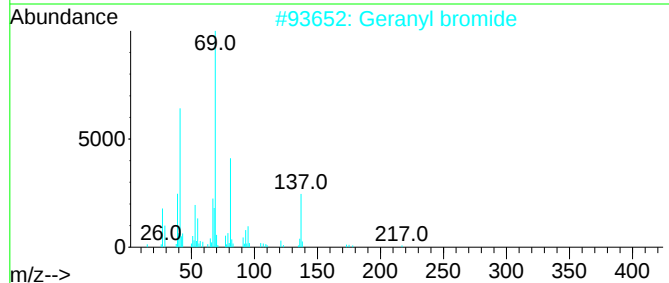
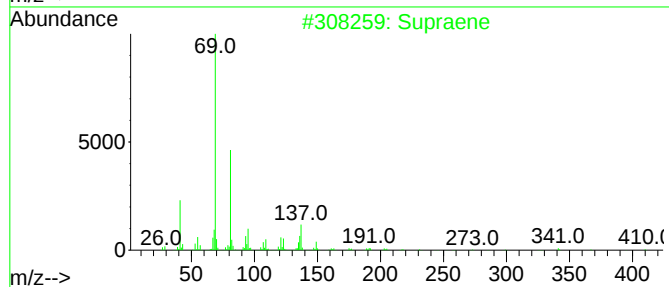
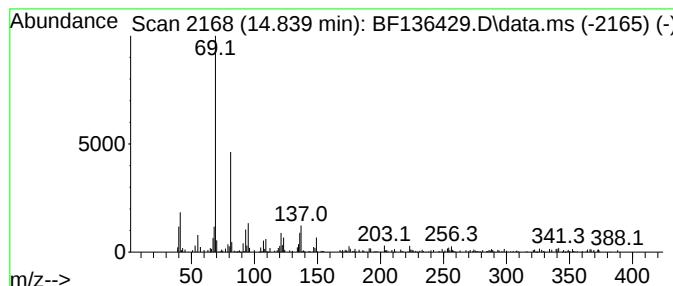
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	3.38 ng	72963	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Geranyl bromide	216	C10H17Br	006138-90-5	72
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136429.D
Acq On : 06 Dec 2023 15:37
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-112223

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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...	9.269	3.2	ng	101066	3	9.828	626576	20.0
Dodecanoic acid...	11.722	2.3	ng	58665	4	11.316	520746	20.0
n-Hexadecanoic ...	11.857	4.2	ng	109552	4	11.316	520746	20.0
9,12-Octadecadi...	12.410	7.8	ng	202351	4	11.316	520746	20.0
9-Octadecenoic ...	12.433	4.9	ng	127324	4	11.316	520746	20.0
Supraene	14.839	3.4	ng	72963	6	15.451	431295	20.0