

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
 Data File : BF135716.D
 Acq On : 11 Oct 2023 16:42
 Operator : CG\JU
 Sample : 04656-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-103S

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: BF135716.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.757	280	284	293	rBV	51080	84382	3.40%	0.600%
2	5.375	556	559	576	rBV	698126	900157	36.23%	6.398%
3	6.392	729	732	751	rBV	415209	581311	23.40%	4.132%
4	6.740	788	791	799	rBV	507356	431058	17.35%	3.064%
5	6.916	818	821	826	rBV2	35853	32908	1.32%	0.234%
6	7.310	884	888	899	rBV	1499004	1517414	61.07%	10.785%
7	7.757	959	964	967	rBV2	79064	71350	2.87%	0.507%
8	7.816	971	974	978	rVB	28725	29261	1.18%	0.208%
9	7.963	992	999	1000	rBV5	15739	27627	1.11%	0.196%
10	8.016	1005	1008	1011	rBV	661288	572952	23.06%	4.072%
11	8.039	1011	1012	1015	rVB	112314	69252	2.79%	0.492%
12	8.528	1092	1095	1098	rBV	51931	36513	1.47%	0.260%
13	8.833	1144	1147	1150	rVB2	45735	37283	1.50%	0.265%
14	9.098	1187	1192	1195	rBV	2756956	2484652	100.00%	17.659%
15	9.216	1210	1212	1218	rVB5	31702	41492	1.67%	0.295%
16	9.775	1303	1307	1310	rBV	724801	596233	24.00%	4.238%
17	9.804	1310	1312	1316	rVB	170194	150253	6.05%	1.068%
18	9.980	1340	1342	1344	rBV3	31245	30406	1.22%	0.216%
19	10.328	1398	1401	1408	rBV	50201	51803	2.08%	0.368%
20	10.575	1439	1443	1455	rBV	1392561	1483437	59.70%	10.543%
21	11.269	1558	1561	1564	rBV	677139	567803	22.85%	4.036%
22	11.292	1564	1565	1570	rVB	88569	69212	2.79%	0.492%
23	11.816	1650	1654	1664	rBV	561153	634529	25.54%	4.510%
24	12.498	1767	1770	1772	rBV	82701	84374	3.40%	0.600%
25	12.521	1772	1774	1780	rVB2	86928	104848	4.22%	0.745%
26	12.598	1784	1787	1795	rVV	579207	614435	24.73%	4.367%
27	12.863	1829	1832	1836	rVB	1512030	1443520	58.10%	10.260%
28	13.327	1908	1911	1919	rVV2	39821	64094	2.58%	0.456%
29	13.392	1920	1922	1928	rVB	50948	64835	2.61%	0.461%
30	13.845	1995	1999	2007	rVB2	87152	170426	6.86%	1.211%
31	13.933	2011	2014	2018	rBV	434391	382000	15.37%	2.715%
32	14.274	2070	2072	2077	rVB2	49578	62863	2.53%	0.447%
33	14.768	2153	2156	2159	rVB	84663	84493	3.40%	0.601%
34	15.404	2260	2264	2271	rBV	372671	492666	19.83%	3.502%

Sum of corrected areas: 14069842

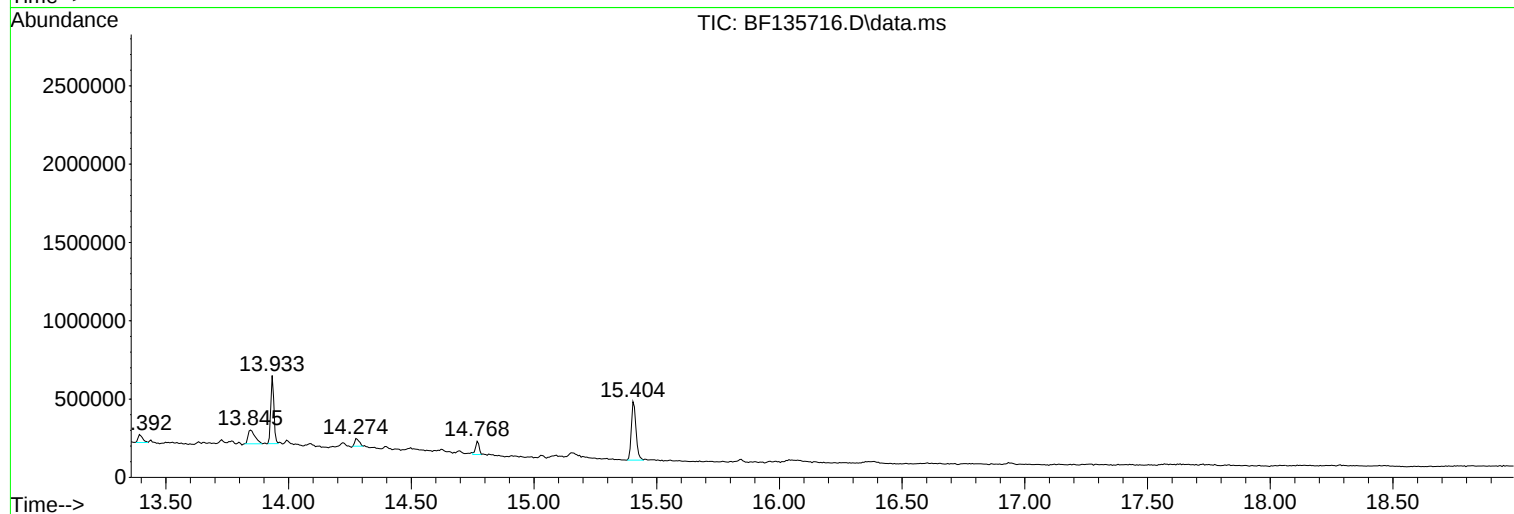
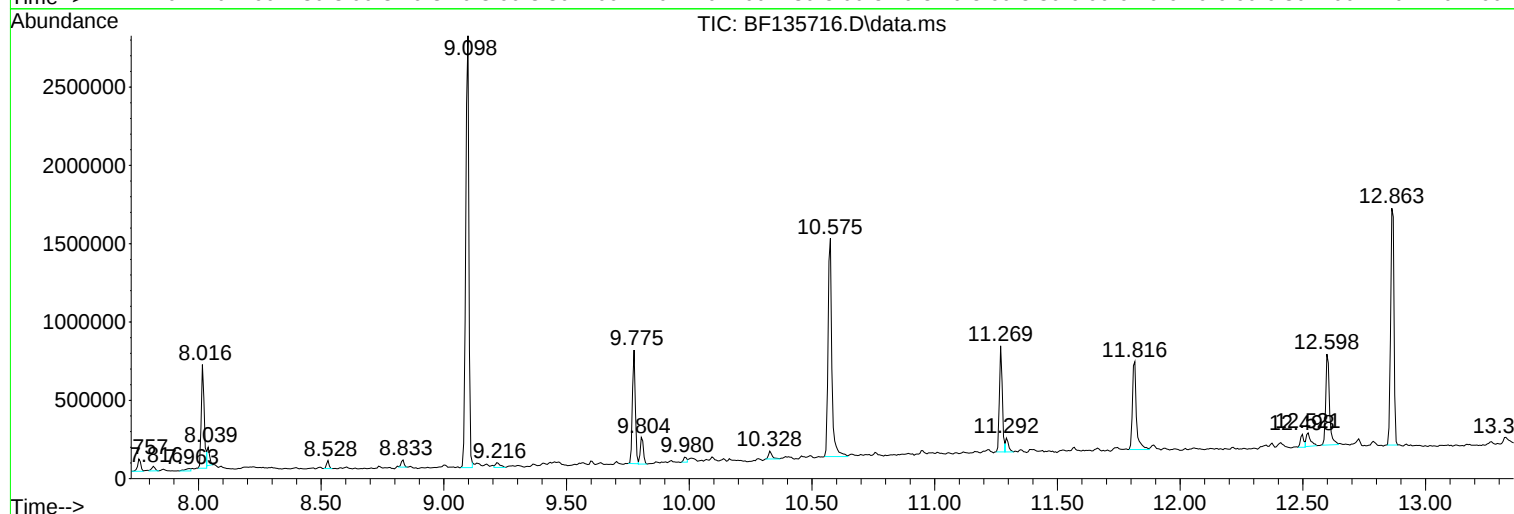
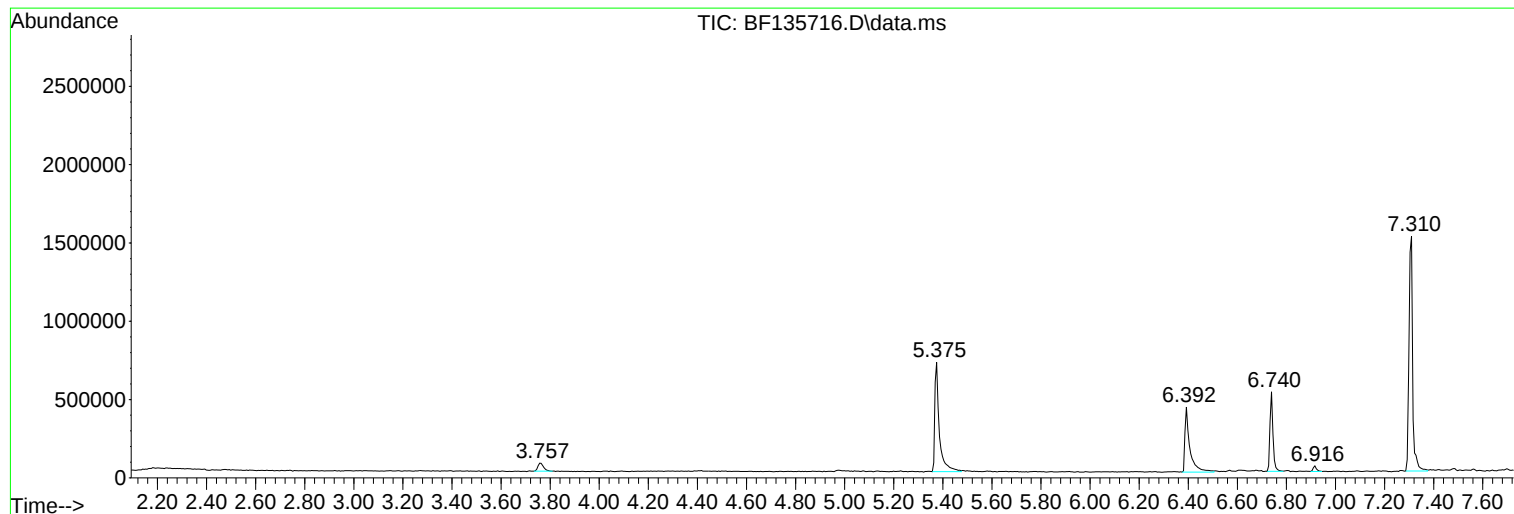
Instrument :
BNA_F
ClientSampleId :
MW-103S

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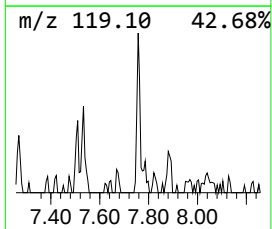
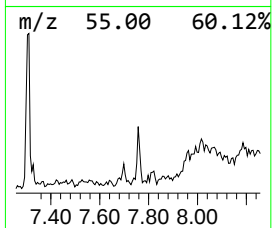
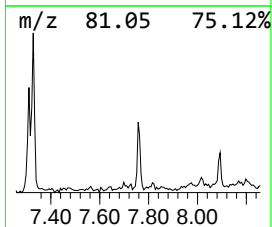
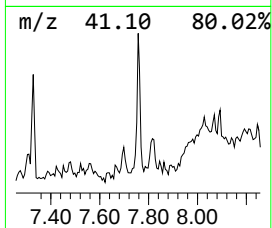
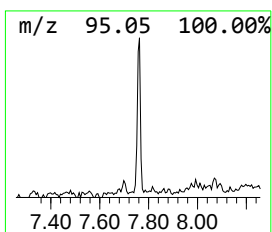
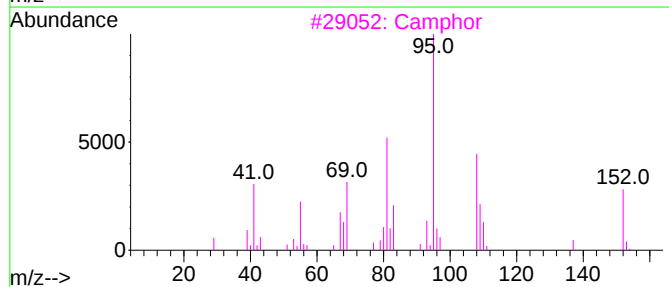
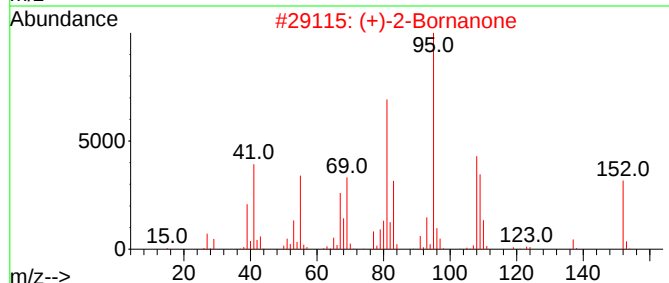
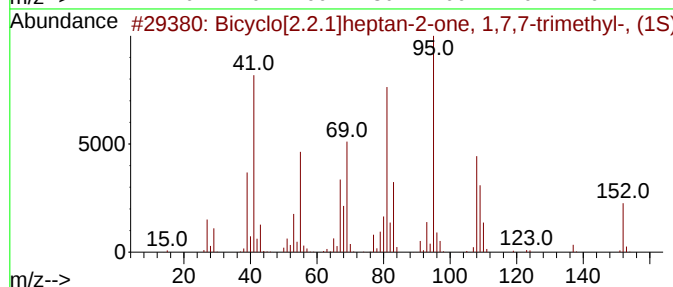
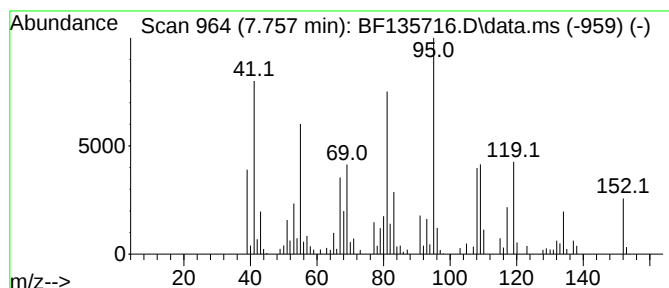
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.757	2.49 ng	71350	Naphthalene-d8	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	93
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	89
3		Camphor	152	C10H16O	000076-22-2	86
4		1,1'-Bicyclopropyl, 2,2,2',2'-te...	138	C10H18	068998-20-9	38
5		Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	38



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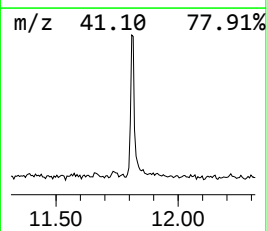
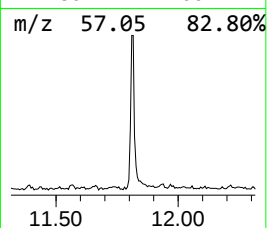
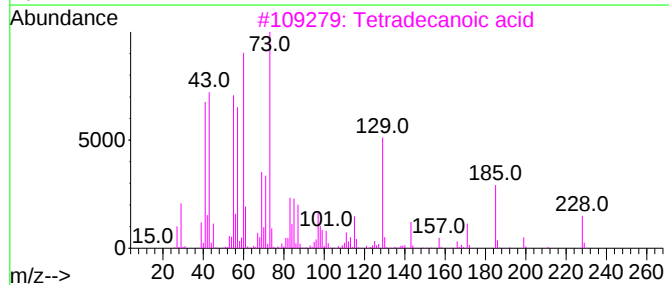
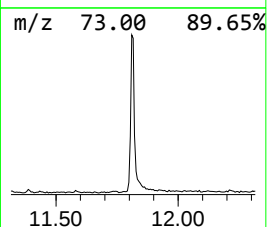
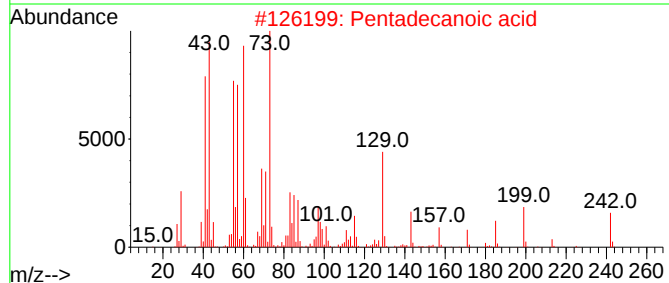
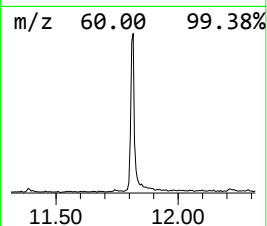
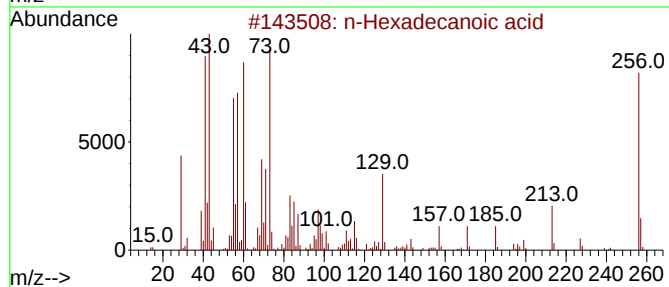
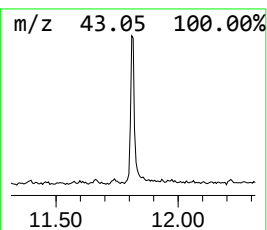
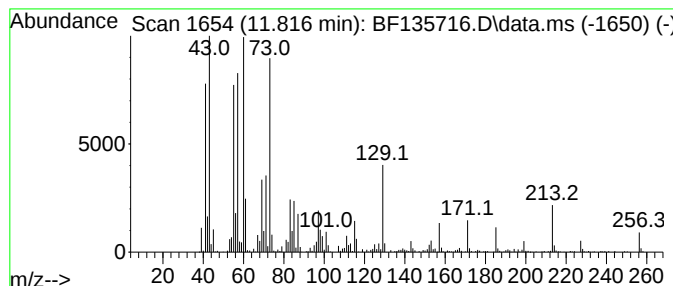
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.816	22.35 ng	634529	Phenanthrene-d10		11.269	
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	90
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
4	Tridecanoic acid		214	C13H26O2	000638-53-9	62
5	n-Decanoic acid		172	C10H20O2	000334-48-5	53



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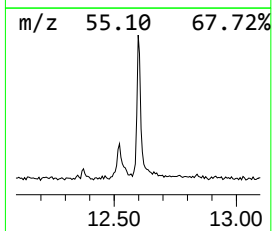
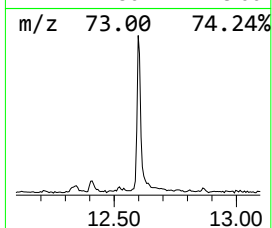
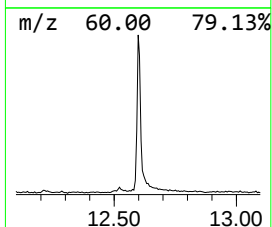
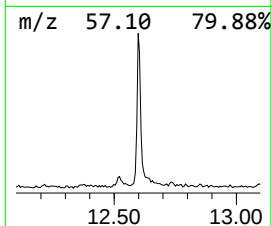
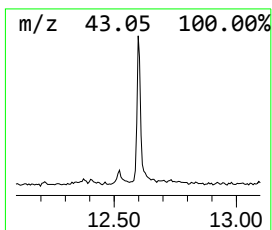
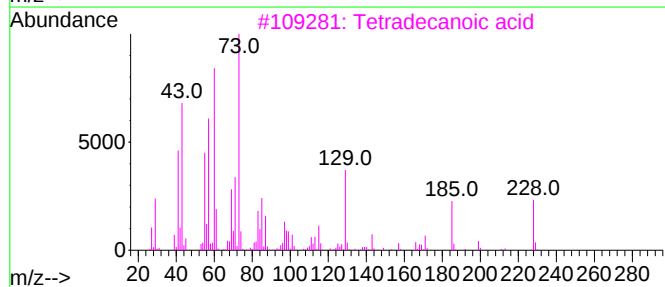
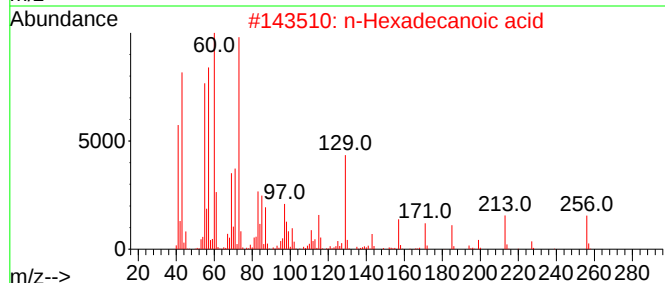
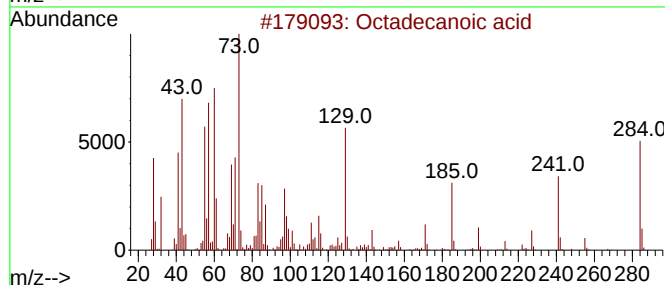
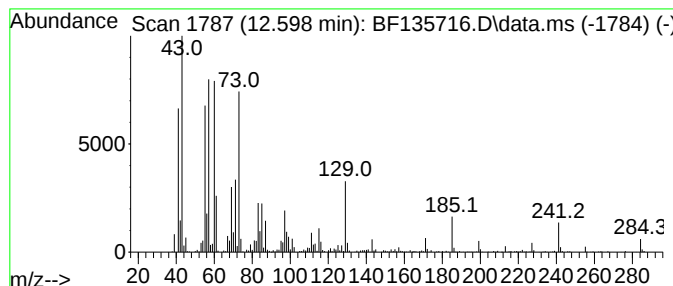
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	21.64 ng	614435	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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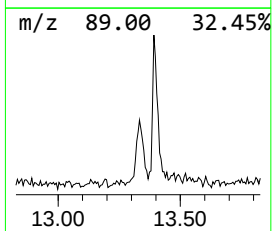
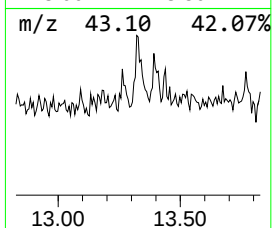
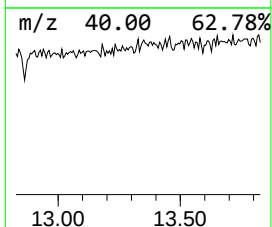
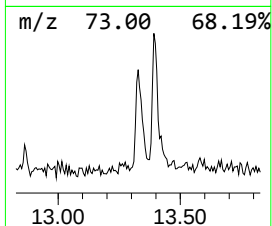
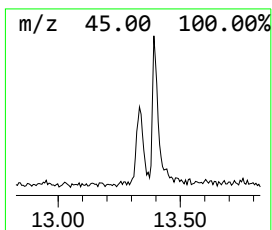
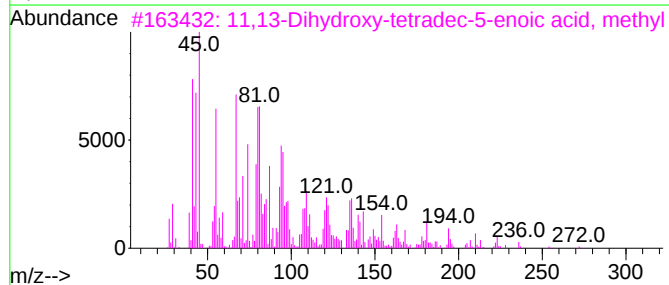
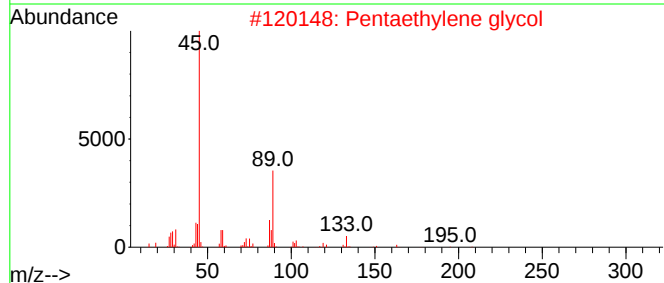
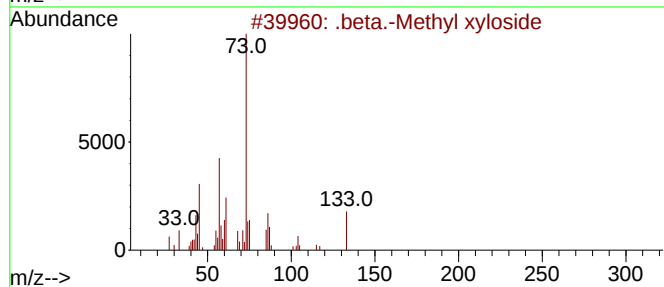
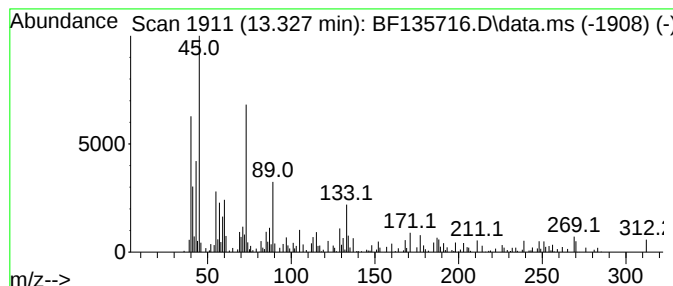
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 .beta.-Methyl xyloside Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	3.36 ng	64094	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Methyl xyloside	164	C6H12O5	007473-45-2	50
2			Pentaethylene glycol	238	C10H22O6	004792-15-8	47
3			11,13-Dihydroxy-tetradec-5-enoic...	272	C15H28O4	1000193-81-4	46
4			1-Nonene, 2-ethyl-3-(methoxymeth...	214	C13H26O2	1000197-21-7	43
5			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	43



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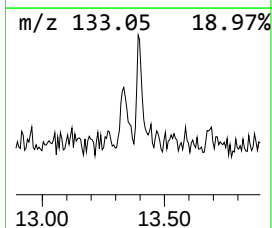
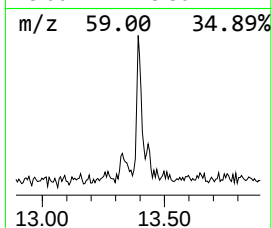
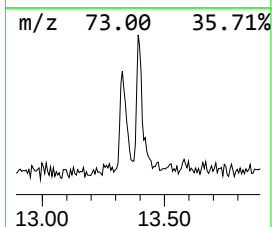
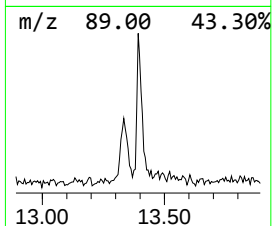
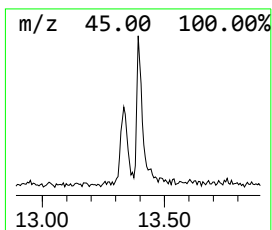
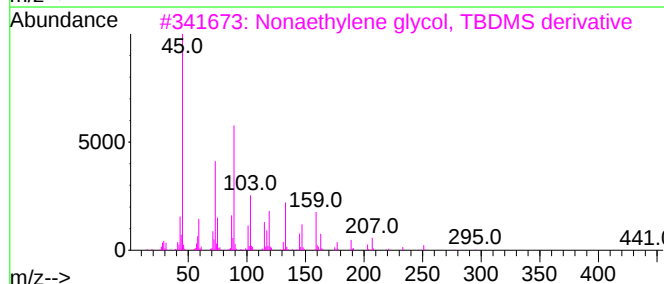
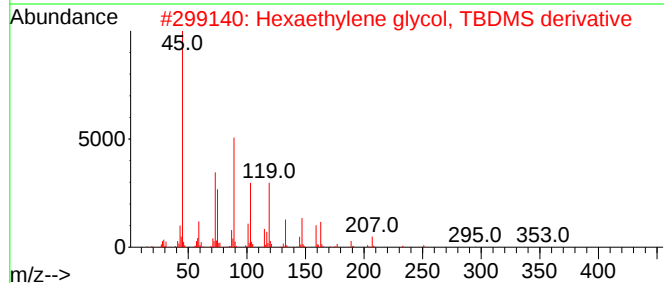
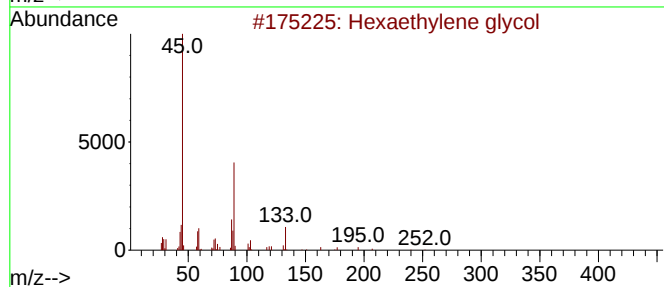
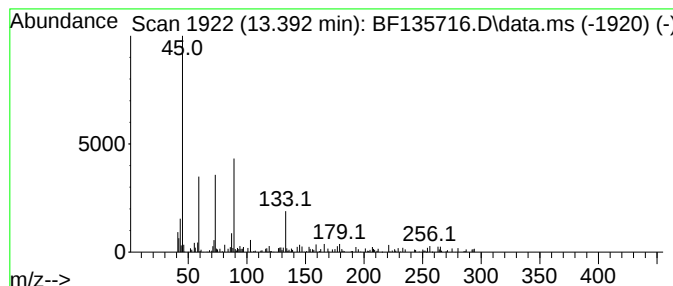
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Hexaethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.392	3.39 ng	64835	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexaethylene glycol	282	C12H26O7	002615-15-8	64
2			Hexaethylene glycol, TBDMS deriv...	396	C18H40O7Si	1000352-11-0	56
3			Nonaethylene glycol, TBDMS deriv...	528	C24H52O10Si	1010352-11-3	56
4			Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	50
5			21-Crown-7	308	C14H28O7	033089-36-0	50



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ClientSampleId :
MW-103S

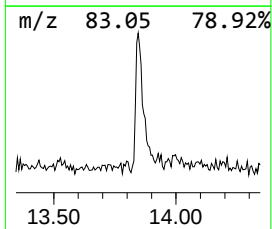
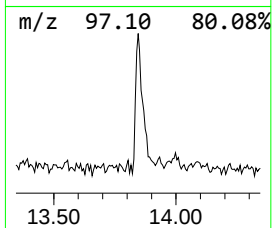
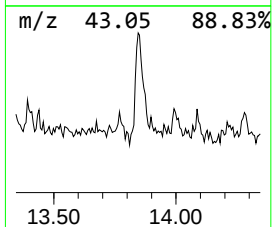
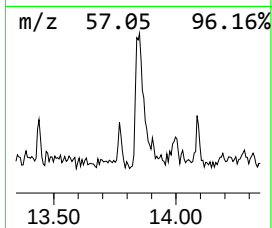
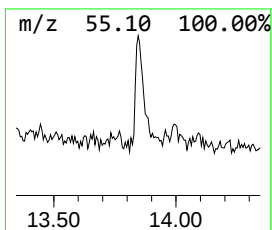
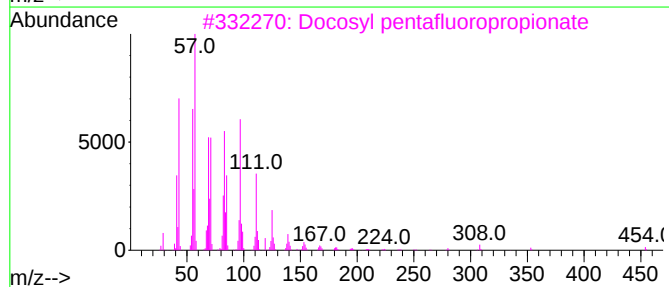
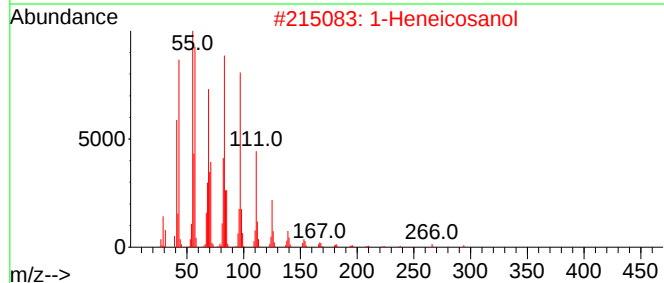
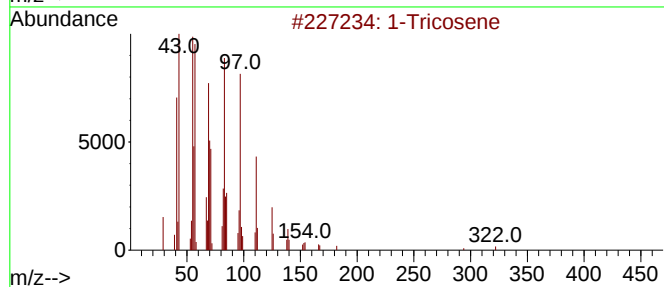
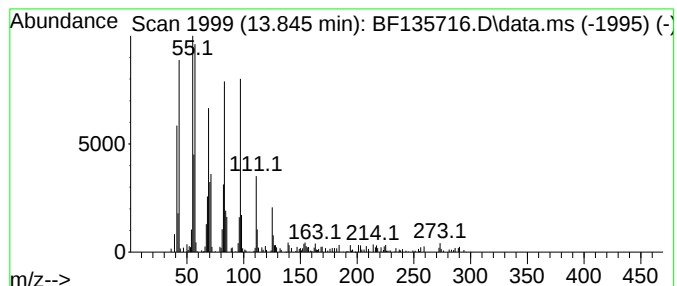
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	8.92 ng	170426	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	91
2	1-Heneicosanol			312	C21H44O	015594-90-8	91
3	Docosyl pentafluoropropionate			472	C25H45F5O2	1000351-80-9	87
4	Octacosanol			410	C28H58O	000557-61-9	87
5	Heptacosyl acetate			438	C29H58O2	1000351-78-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135716.D
Acq On : 11 Oct 2023 16:42
Operator : CG\JU
Sample : 04656-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103S

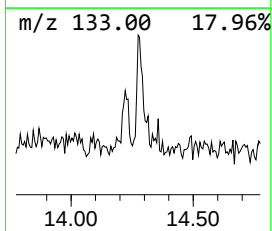
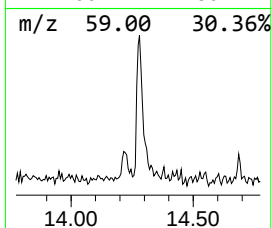
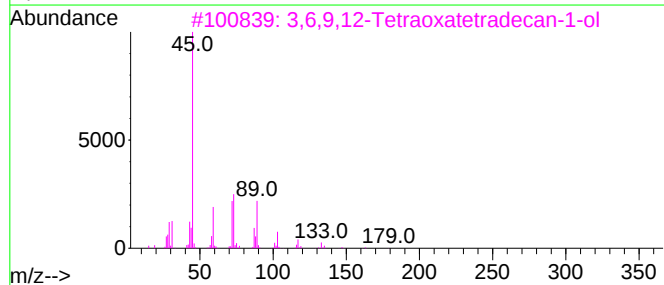
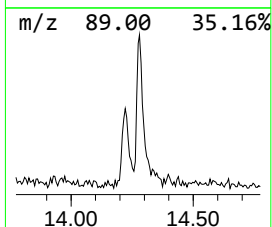
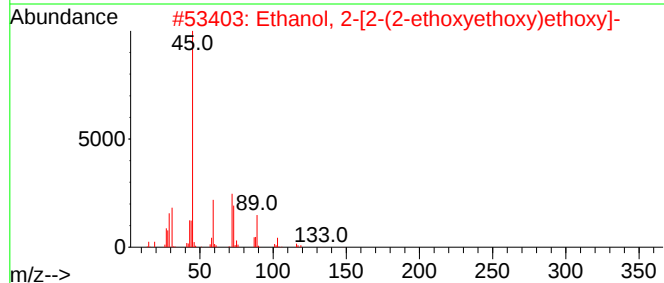
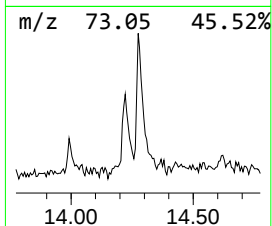
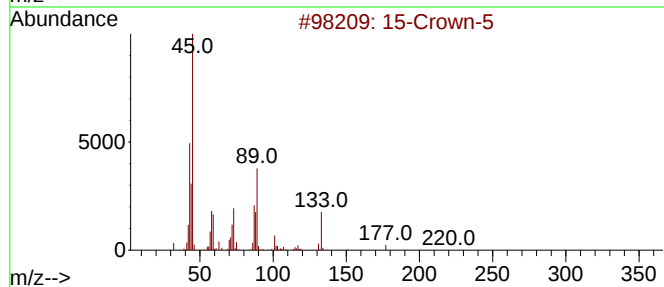
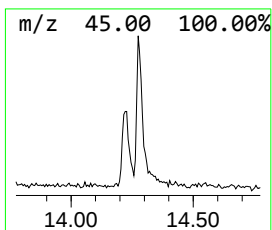
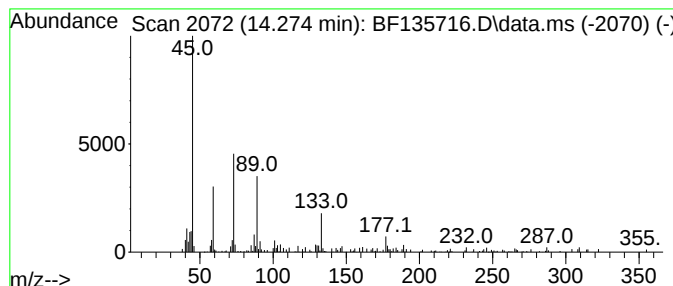
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 15-Crown-5 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	3.29 ng	62863	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Crown-5			220	C10H20O5	033100-27-5	72
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...			178	C8H18O4	000112-50-5	72
3	3,6,9,12-Tetraoxatetradecan-1-ol			222	C10H22O5	005650-20-4	64
4	Acetaldehyde, tetramer			176	C8H16O4	000108-62-3	50
5	Butanoic acid, 4-methoxy-			118	C5H10O3	029006-02-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135716.D
Acq On : 11 Oct 2023 16:42
Operator : CG\JU
Sample : 04656-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103S

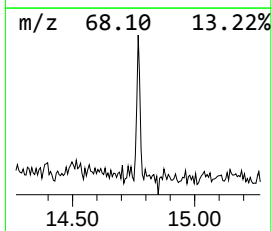
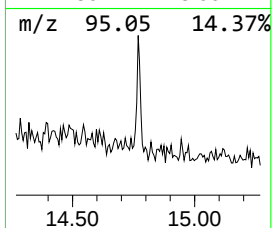
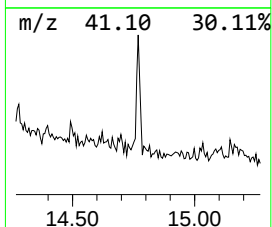
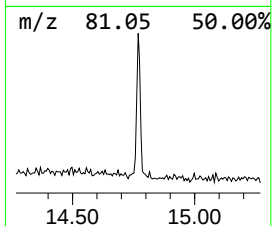
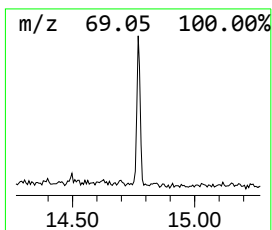
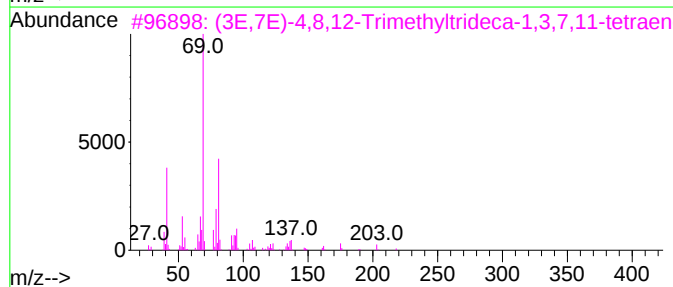
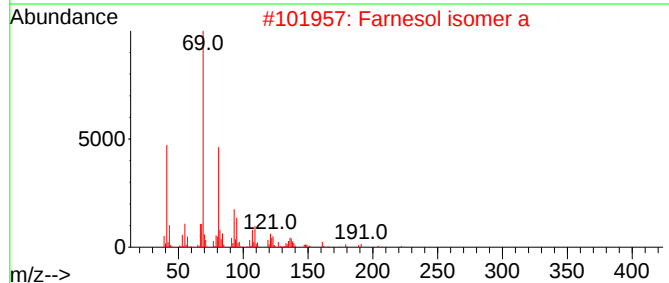
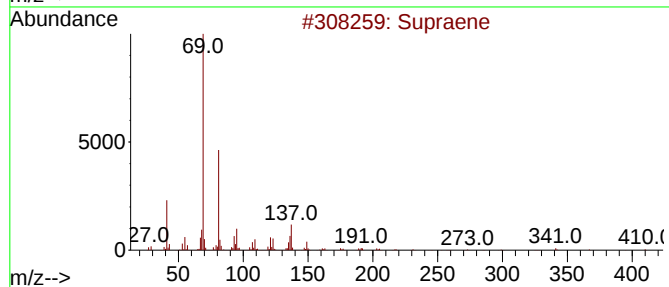
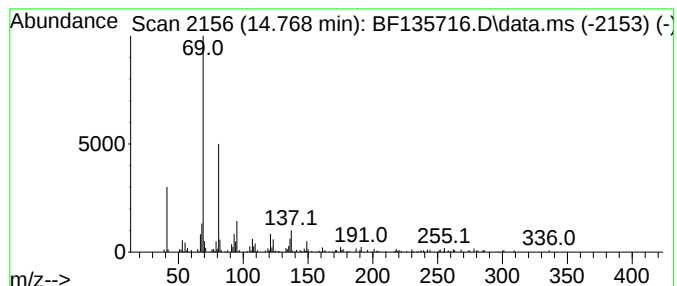
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	3.43 ng	84493	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Farnesol isomer a	222	C15H26O	1000108-92-4	76
3			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	74
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101123\
Data File : BF135716.D
Acq On : 11 Oct 2023 16:42
Operator : CG\JU
Sample : 04656-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
Bicyclo[2.2.1]h...	7.757	2.5	ng	71350	2	8.016	572952	20.0
n-Hexadecanoic ...	11.816	22.4	ng	634529	4	11.269	567803	20.0
Octadecanoic acid	12.598	21.6	ng	614435	4	11.269	567803	20.0
.beta.-Methyl x...	13.327	3.4	ng	64094	5	13.933	382000	20.0
Hexaethylene gl...	13.392	3.4	ng	64835	5	13.933	382000	20.0
1-Tricosene	13.845	8.9	ng	170426	5	13.933	382000	20.0
15-Crown-5	14.274	3.3	ng	62863	5	13.933	382000	20.0
Supraene	14.768	3.4	ng	84493	6	15.404	492666	20.0