

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
 Data File : BF135211.D
 Acq On : 13 Sep 2023 07:38
 Operator : CG\JU
 Sample : 04293-01
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SOIL

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: BF135211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	24834	31338	2.00%	0.229%
2	4.987	490	493	501	rBV	53030	60658	3.87%	0.443%
3	5.387	557	561	579	rBV	1611156	1541348	98.42%	11.263%
4	6.398	729	733	736	rBV	1651512	1566053	100.00%	11.444%
5	6.598	764	767	773	rBV	20184	29769	1.90%	0.218%
6	6.763	791	795	798	rBV	945024	749163	47.84%	5.474%
7	7.322	886	890	894	rBV	1049147	957677	61.15%	6.998%
8	8.040	1008	1012	1016	rBV	1181388	976101	62.33%	7.133%
9	9.116	1191	1195	1199	rBV	1561446	1320624	84.33%	9.650%
10	9.239	1212	1216	1220	rVB	32470	31378	2.00%	0.229%
11	9.798	1307	1311	1314	rBV	1232543	997663	63.71%	7.290%
12	10.586	1441	1445	1456	rBV	920912	779495	49.77%	5.696%
13	11.286	1561	1564	1568	rBV	1045090	906928	57.91%	6.627%
14	11.351	1572	1575	1579	rVB4	14390	15979	1.02%	0.117%
15	11.827	1652	1656	1666	rBV	238554	251008	16.03%	1.834%
16	12.504	1769	1771	1775	rBV	18406	25567	1.63%	0.187%
17	12.551	1775	1779	1786	rVB5	14907	27830	1.78%	0.203%
18	12.616	1786	1790	1800	rBV2	57684	78434	5.01%	0.573%
19	12.710	1803	1806	1809	rBV2	35341	32407	2.07%	0.237%
20	12.786	1817	1819	1825	rVB2	21110	21460	1.37%	0.157%
21	12.880	1832	1835	1839	rBV	1042022	952288	60.81%	6.959%
22	13.122	1870	1876	1880	rBV	29120	47036	3.00%	0.344%
23	13.316	1907	1909	1912	rBV3	21885	21880	1.40%	0.160%
24	13.469	1931	1935	1937	rBV2	30956	30884	1.97%	0.226%
25	13.798	1988	1991	1993	rBV	39338	39862	2.55%	0.291%
26	13.821	1993	1995	2009	rVB4	61329	143503	9.16%	1.049%
27	13.945	2011	2016	2019	rBV	630829	640118	40.87%	4.678%
28	14.116	2042	2045	2049	rVB	35799	31774	2.03%	0.232%
29	14.421	2094	2097	2102	rBV	39878	44648	2.85%	0.326%
30	14.727	2147	2149	2153	rVB	31835	29618	1.89%	0.216%
31	14.804	2159	2162	2165	rBV	21923	22780	1.45%	0.166%
32	14.980	2189	2192	2199	rVB4	30339	53578	3.42%	0.392%
33	15.068	2204	2207	2212	rVB	52519	60693	3.88%	0.444%
34	15.339	2251	2253	2259	rVB2	19911	29646	1.89%	0.217%
35	15.410	2259	2265	2269	rBV	499764	650523	41.54%	4.754%
36	15.892	2342	2347	2351	rBV2	36145	58456	3.73%	0.427%

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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	17.504	2615	2621	2622	rBV4	64738	91341	5.83%	0.667%
38	17.974	2695	2701	2703	rBV5	24042	56652	3.62%	0.414%
39	18.027	2704	2710	2723	rVB5	83095	278513	17.78%	2.035%

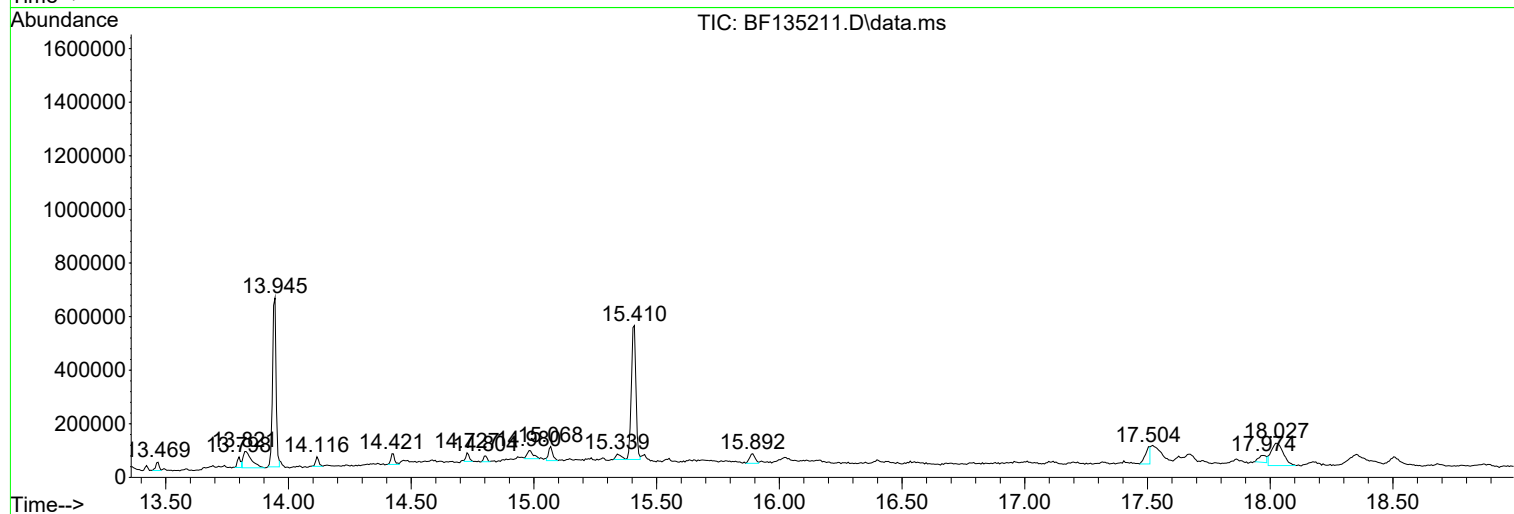
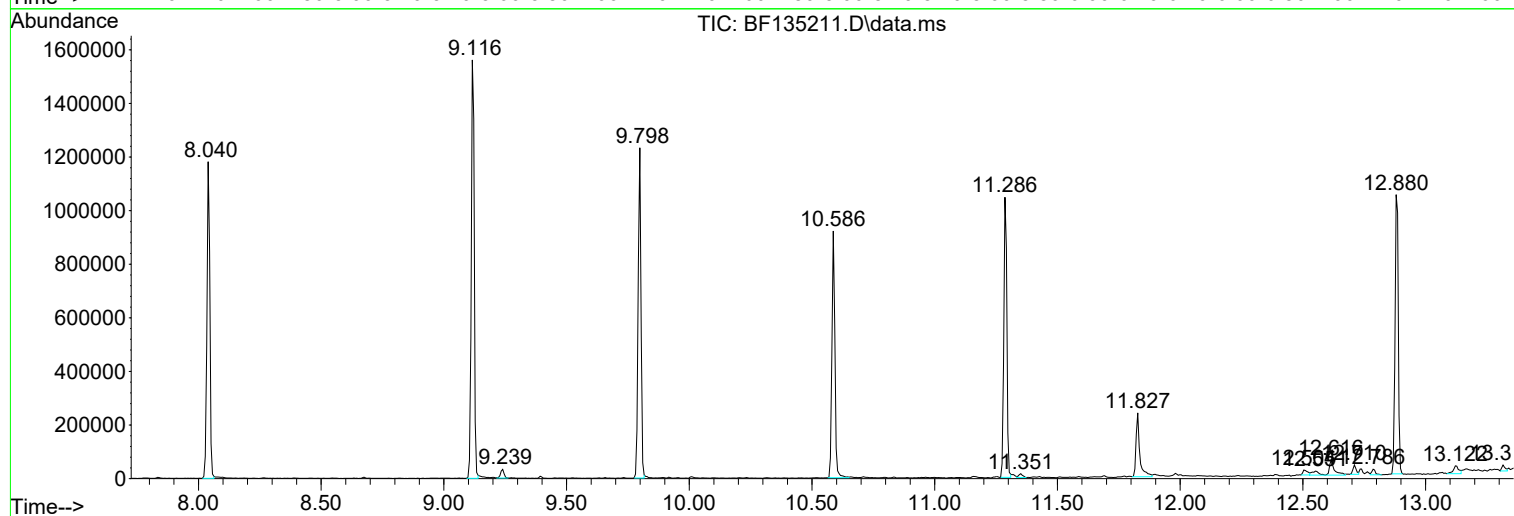
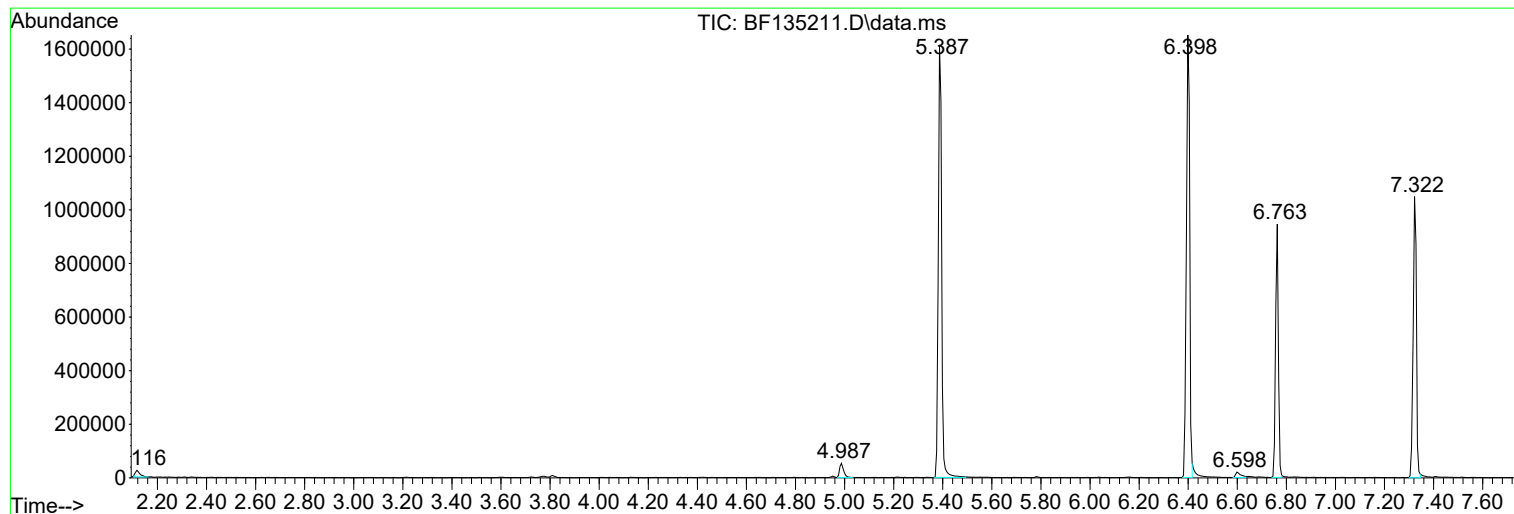
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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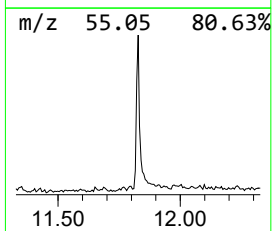
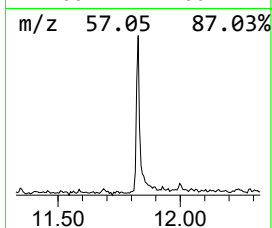
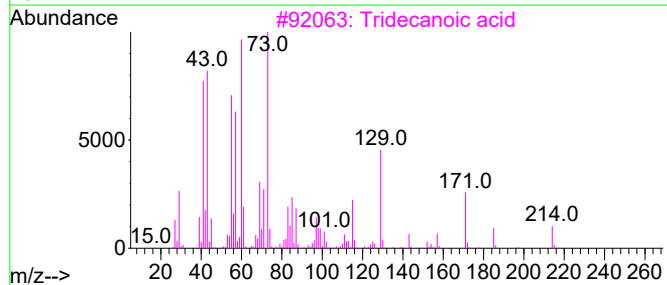
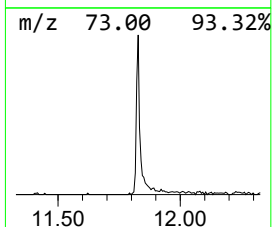
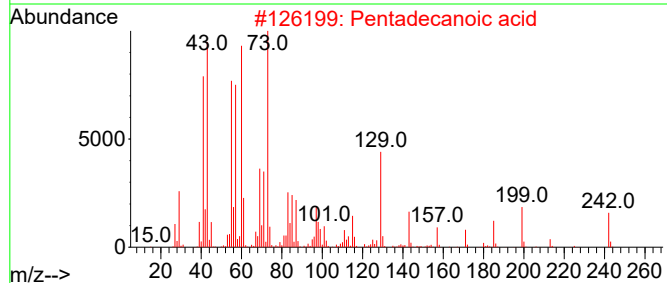
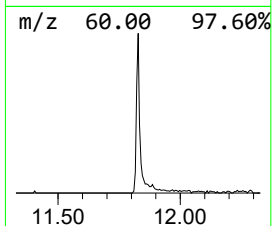
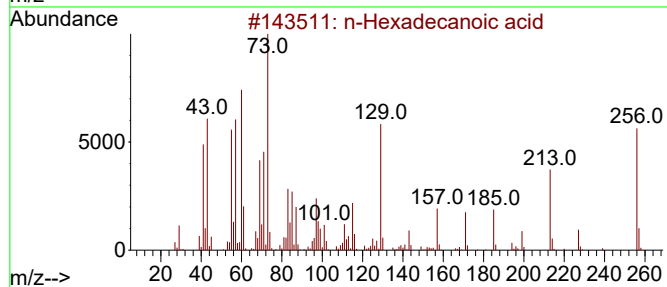
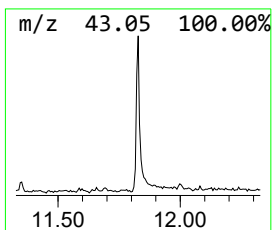
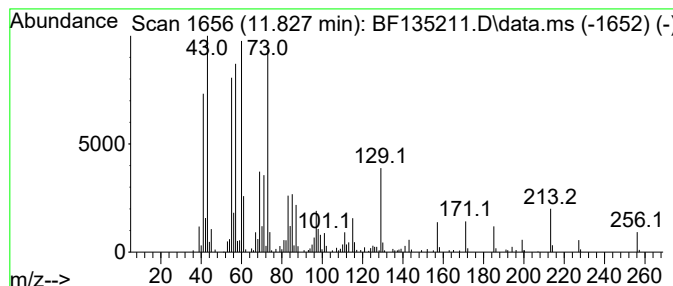
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.828	5.54 ng	251008	Phenanthrene-d10		11.286	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	n-Decanoic acid		172	C10H20O2	000334-48-5	60



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Instrument :
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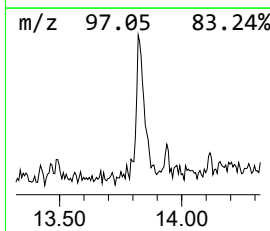
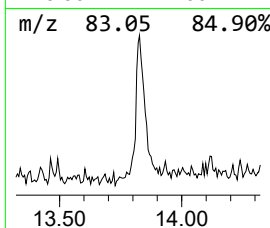
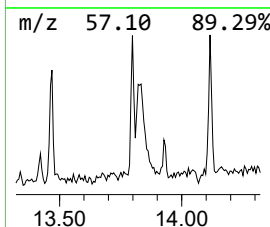
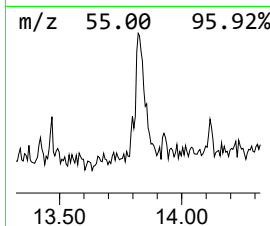
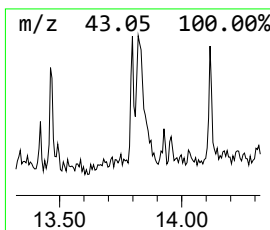
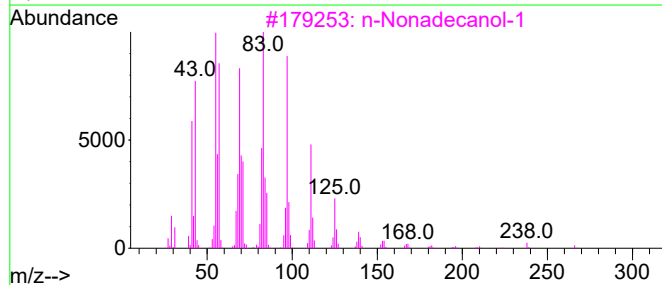
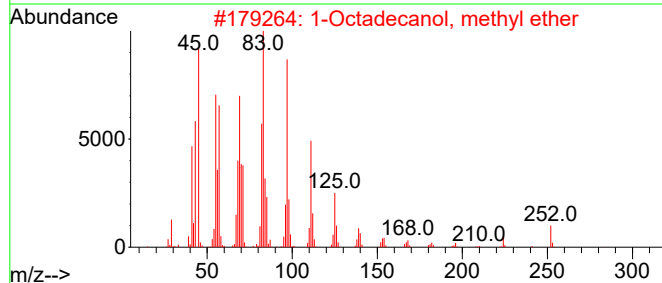
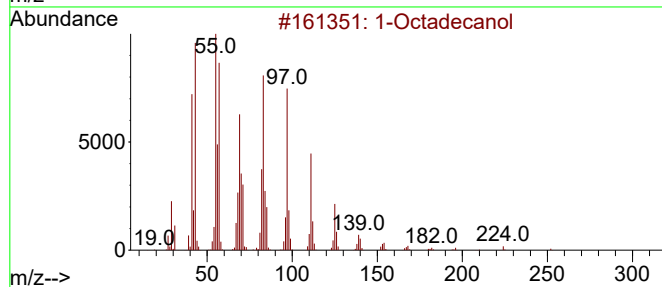
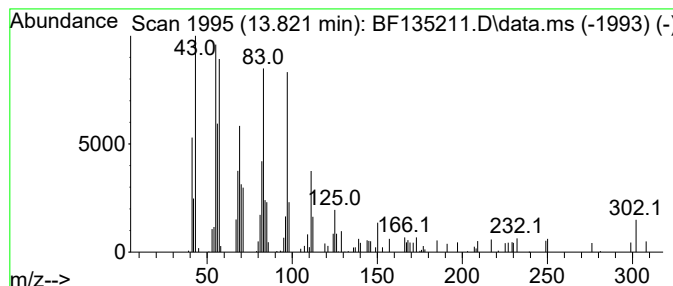
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 1-Octadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	4.48 ng	143503	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	91
2			1-Octadecanol, methyl ether	284	C19H40O	1000406-29-3	90
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
4			Behenic alcohol	326	C22H46O	000661-19-8	87
5			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	87



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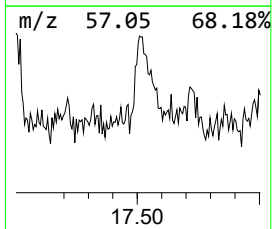
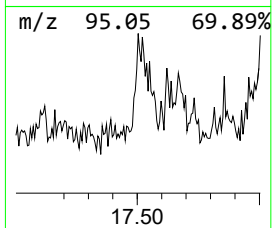
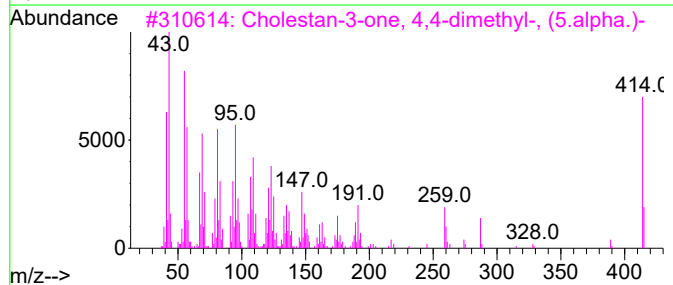
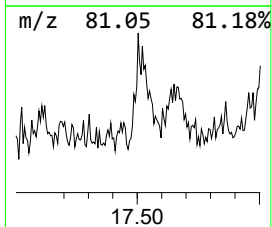
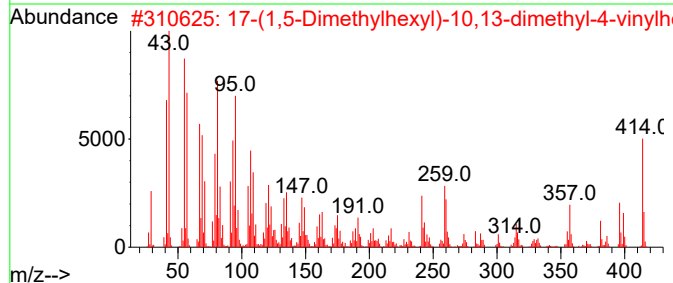
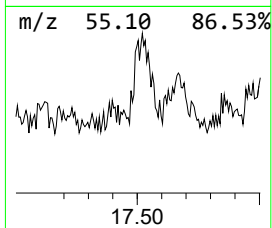
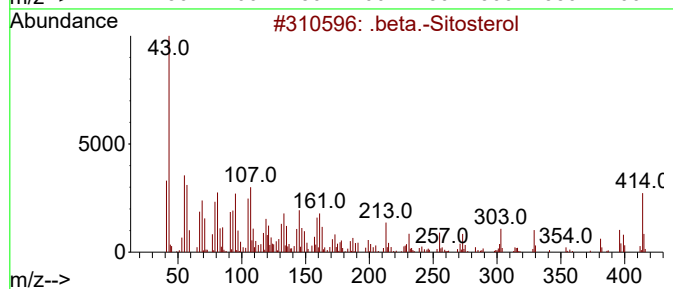
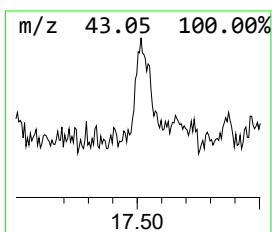
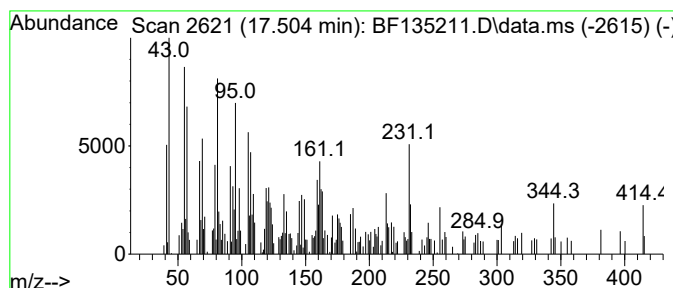
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 .beta.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.504	2.81 ng	91341	Perylene-d12	15.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	64
2	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	53
3	Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	52
4	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	38
5	(1S,3E,7E,11E)-Cembra-3,7,11-triene	274	C20H34	1000432-97-5	30



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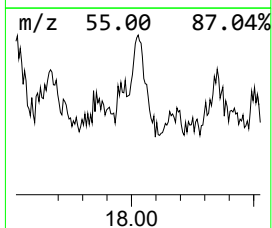
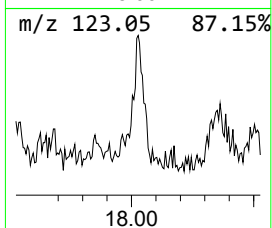
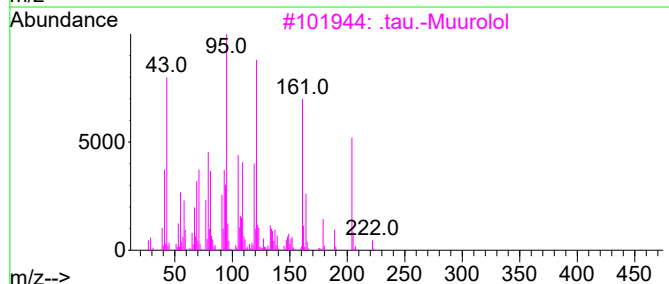
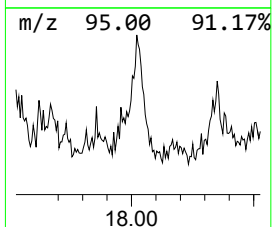
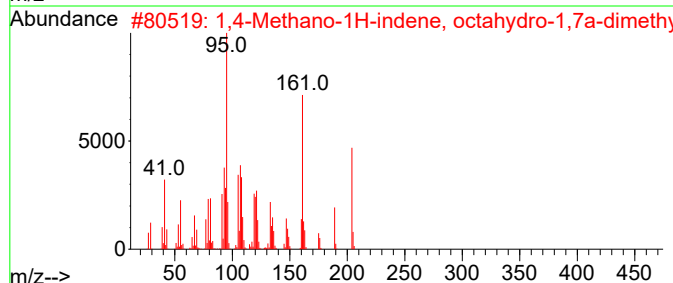
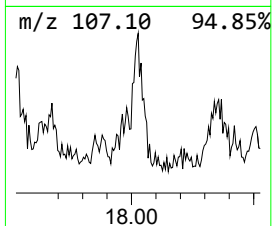
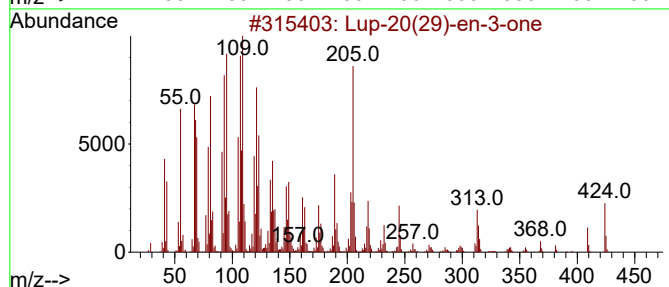
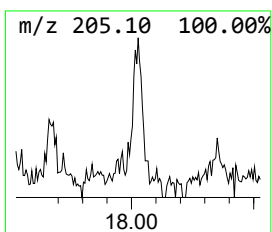
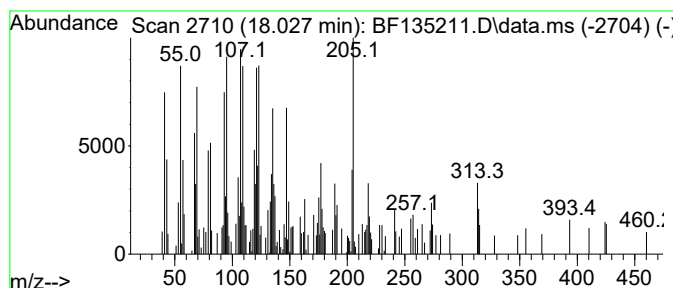
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Lup-20(29)-en-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.027	8.56 ng	278513	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	72
2			1,4-Methano-1H-indene, octahydro...	204	C15H24	087064-18-4	25
3			.tau.-Muurolol	222	C15H26O	019912-62-0	22
4			1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	16
5			Benzamide, 4-fluoro-N-(2H-[1,2,4...	273	C13H8FN3OS	1000350-88-5	14



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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 ...	11.828	5.5	ng	251008	4	11.286	906928	20.0
1-Octadecanol	13.822	4.5	ng	143503	5	13.945	640118	20.0
.beta.-Sitosterol	17.504	2.8	ng	91341	6	15.410	650523	20.0
Lup-20(29)-en-3...	18.027	8.6	ng	278513	6	15.410	650523	20.0