

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
 Data File : BF129489.D
 Acq On : 01 Aug 2022 23:38
 Operator : CG\JU
 Sample : N3896-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RVE-64

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129489.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	478	481	491	rVB	40847	53448	1.29%	0.172%
2	5.516	545	549	552	rBV	4193877	3773074	91.20%	12.116%
3	6.522	715	720	723	rBV	4134255	3669928	88.71%	11.785%
4	6.875	776	780	783	rBV	1149317	905100	21.88%	2.906%
5	7.440	871	876	879	rBV	2730032	2445383	59.11%	7.853%
6	8.157	994	998	1001	rBV	1344973	1128244	27.27%	3.623%
7	9.228	1176	1180	1184	rBV	4469769	4137112	100.00%	13.285%
8	9.910	1292	1296	1300	rBV	1276996	1065642	25.76%	3.422%
9	10.704	1427	1431	1434	rBV	2170381	1811417	43.78%	5.817%
10	11.404	1546	1550	1552	rBV	875557	841623	20.34%	2.703%
11	11.422	1552	1553	1558	rVV	209518	175944	4.25%	0.565%
12	11.475	1558	1562	1565	rVB	54022	50071	1.21%	0.161%
13	11.780	1611	1614	1618	rVB	86736	65316	1.58%	0.210%
14	12.486	1730	1734	1737	rVB3	64399	57112	1.38%	0.183%
15	12.616	1752	1756	1760	rBV	455425	367277	8.88%	1.179%
16	12.827	1789	1792	1793	rBV2	74705	74761	1.81%	0.240%
17	12.845	1793	1795	1801	rVB	378256	319529	7.72%	1.026%
18	12.986	1811	1819	1822	rBV	3507371	3046962	73.65%	9.784%
19	13.069	1827	1833	1836	rBV2	33487	63527	1.54%	0.204%
20	13.274	1864	1868	1871	rVB3	43564	63801	1.54%	0.205%
21	13.680	1934	1937	1942	rVB	91040	89473	2.16%	0.287%
22	13.792	1952	1956	1959	rBV2	53143	66126	1.60%	0.212%
23	13.874	1966	1970	1980	rBV3	300009	568502	13.74%	1.826%
24	14.045	1994	1999	2001	rBV2	1092345	1152284	27.85%	3.700%
25	14.069	2001	2003	2009	rVB	265120	239084	5.78%	0.768%
26	14.133	2011	2014	2019	rBV3	40348	60157	1.45%	0.193%
27	14.316	2042	2045	2048	rVB2	46740	44500	1.08%	0.143%
28	14.427	2062	2064	2068	rVB	60533	58140	1.41%	0.187%
29	14.516	2073	2079	2088	rBV4	271663	639534	15.46%	2.054%
30	14.880	2138	2141	2145	rVB	50506	51534	1.25%	0.165%
31	14.951	2150	2153	2156	rVB	79980	78229	1.89%	0.251%
32	15.092	2173	2177	2180	rBV	273696	402177	9.72%	1.291%
33	15.139	2183	2185	2189	rVB	183398	200718	4.85%	0.645%
34	15.404	2226	2230	2234	rVB	156064	201107	4.86%	0.646%
35	15.463	2236	2240	2245	rVB	204700	248769	6.01%	0.799%
36	15.527	2246	2251	2255	rBV	807261	1011197	24.44%	3.247%

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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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.733	2283	2286	2293	rVB	119569	165808	4.01%	0.532%
38	15.968	2322	2326	2331	rVB	131312	182465	4.41%	0.586%
39	16.780	2459	2464	2469	rBV3	123850	222765	5.38%	0.715%
40	17.027	2501	2506	2511	rBV2	73132	154489	3.73%	0.496%
41	17.180	2527	2532	2542	rBV8	90503	268324	6.49%	0.862%
42	17.686	2614	2618	2628	rVB6	154270	337191	8.15%	1.083%
43	18.462	2743	2750	2774	rVB6	106519	583422	14.10%	1.873%

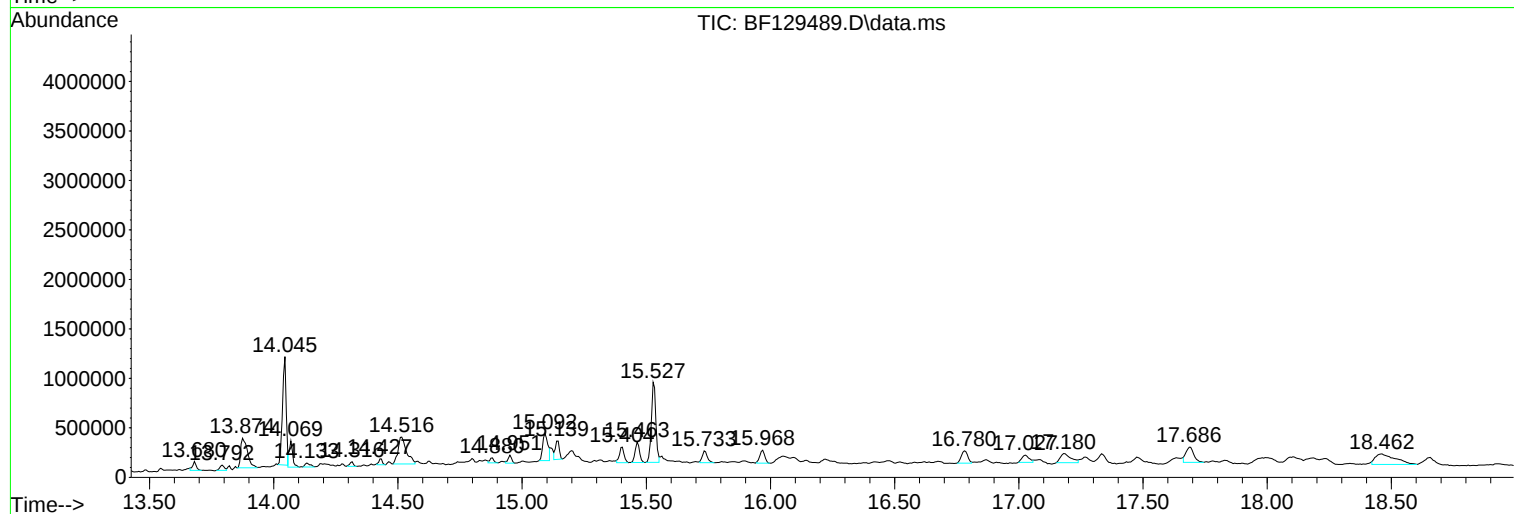
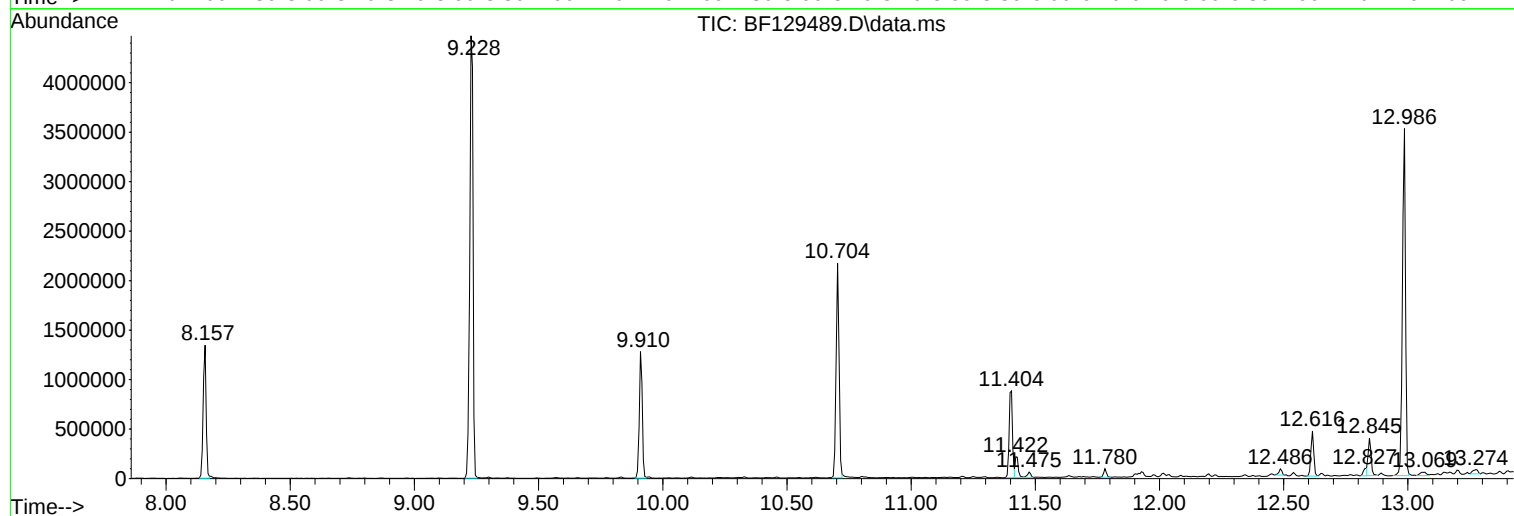
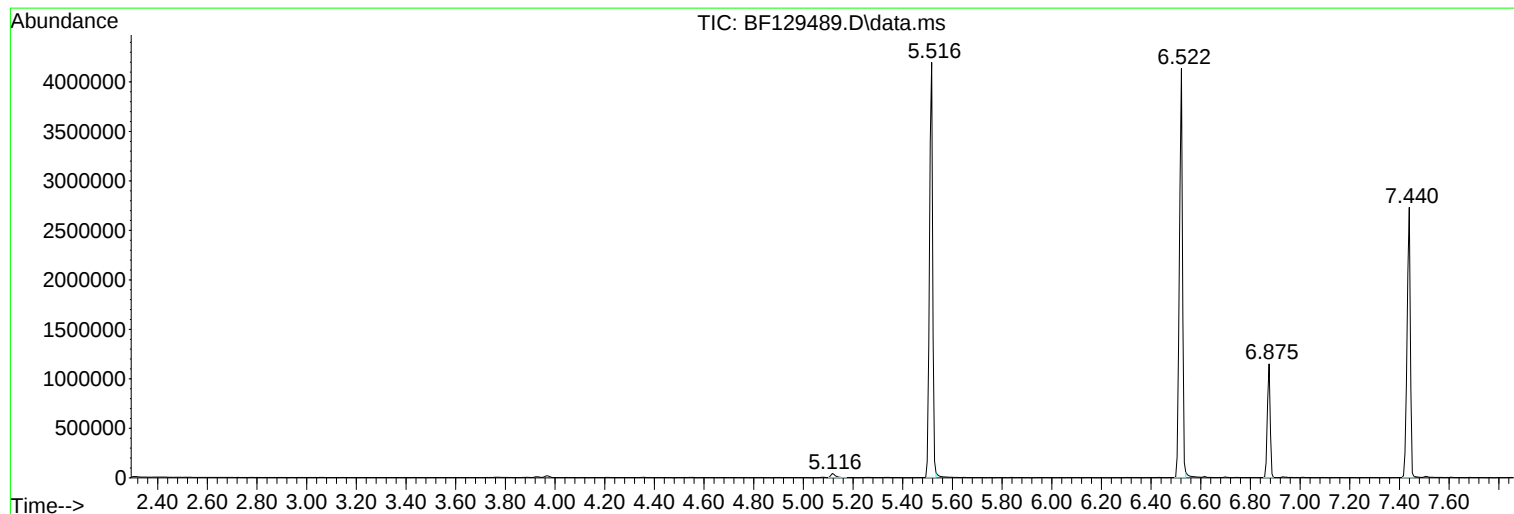
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 15 Sample Multiplier: 1

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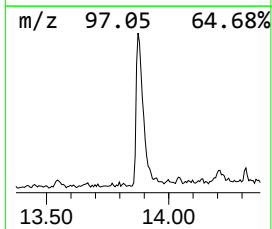
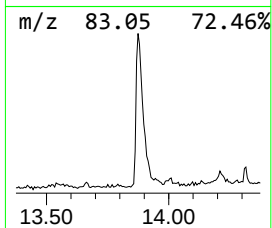
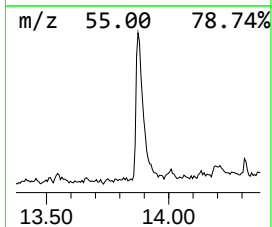
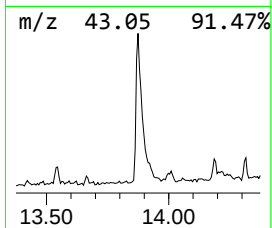
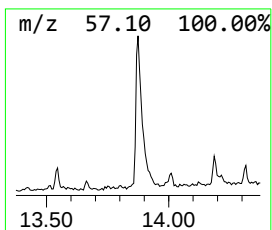
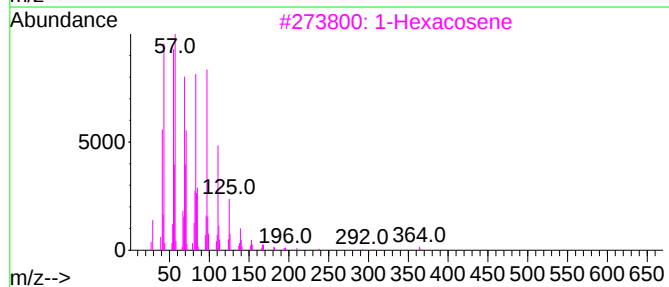
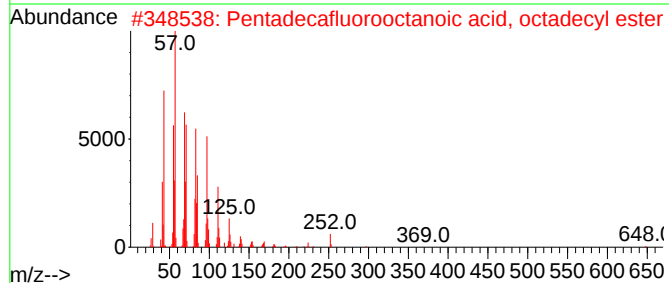
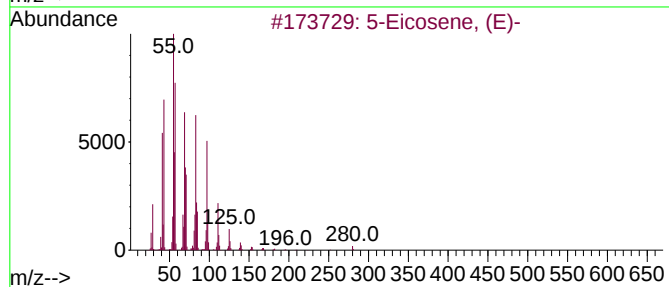
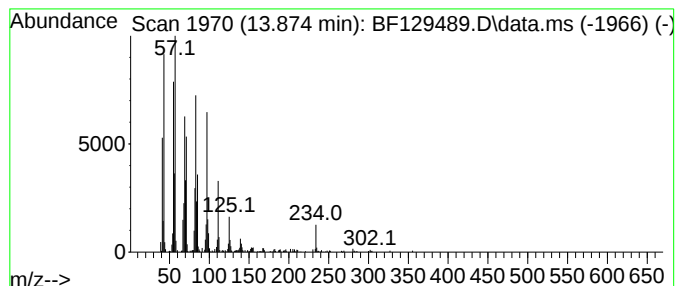
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	9.87 ng	568502	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3		1-Hexacosene	364	C26H52	018835-33-1	94
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	93
5		Cyclopentadecane	210	C15H30	000295-48-7	93



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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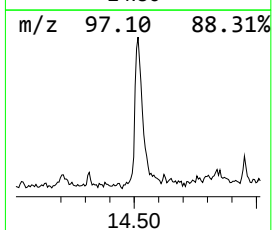
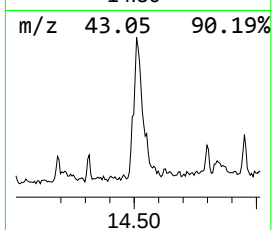
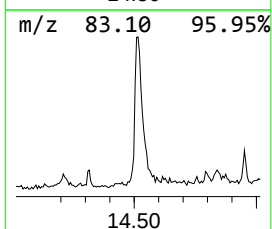
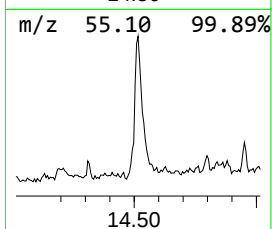
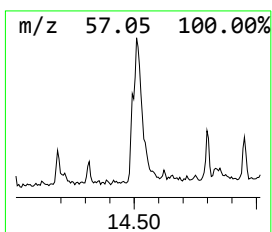
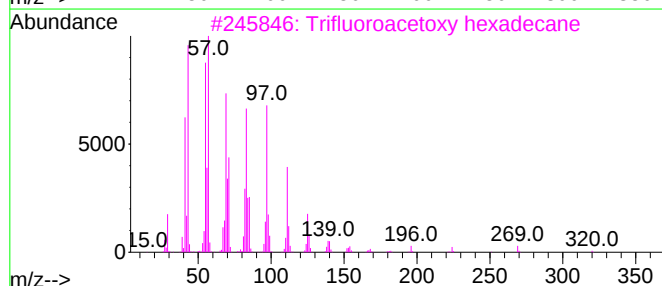
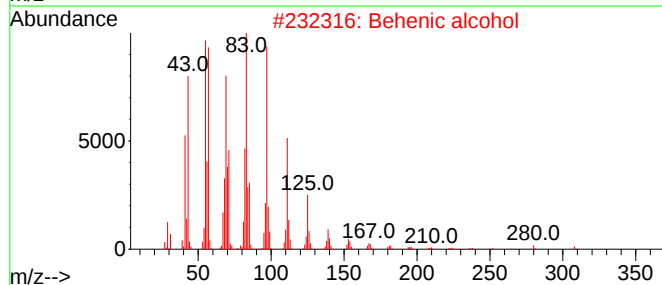
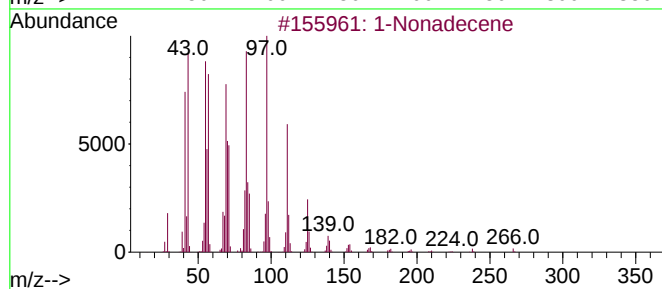
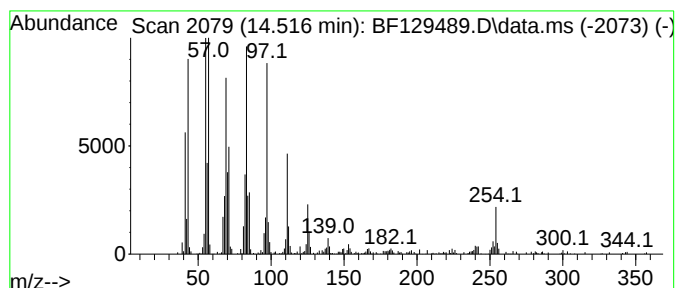
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.516	11.10 ng	639534	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	96
2	Behenic alcohol			326	C22H46O	000661-19-8	94
3	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
4	Pentacos-1-ene			350	C25H50	016980-85-1	94
5	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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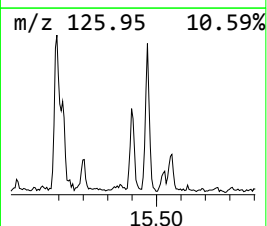
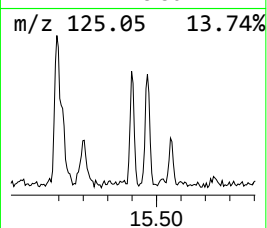
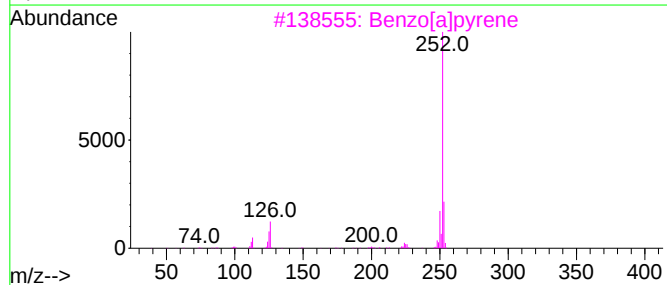
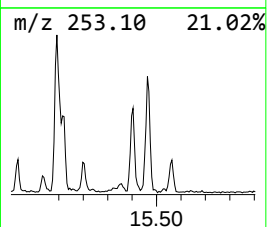
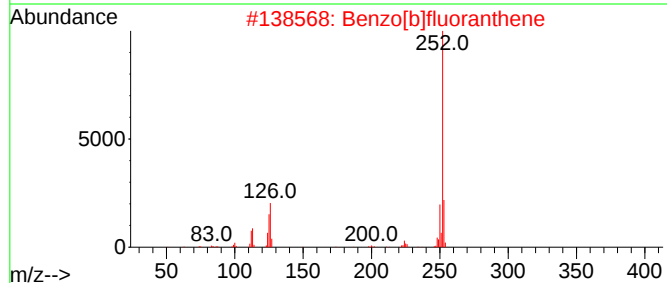
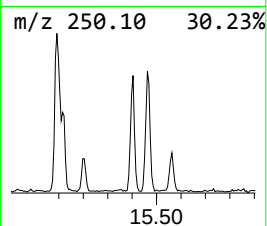
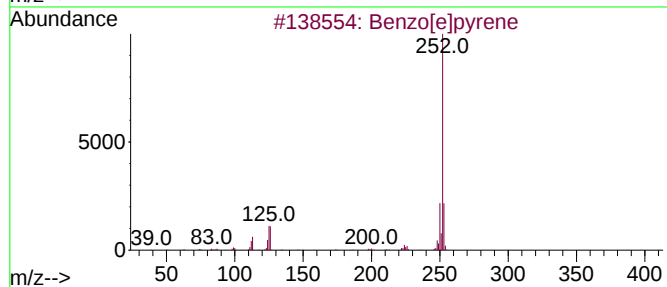
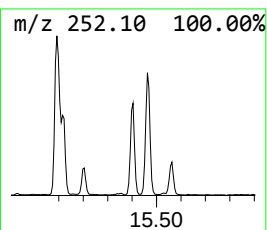
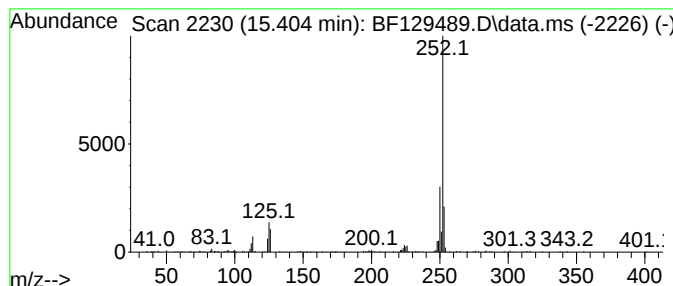
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	3.98 ng	201107	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[a]pyrene	252	C20H12	000050-32-8	96
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5			Perylene	252	C20H12	000198-55-0	90



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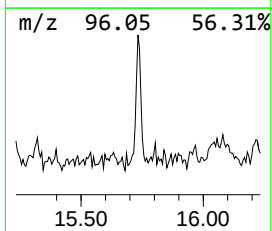
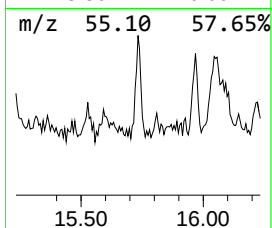
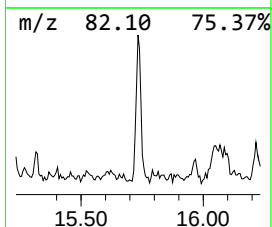
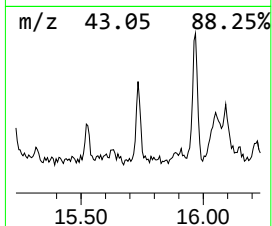
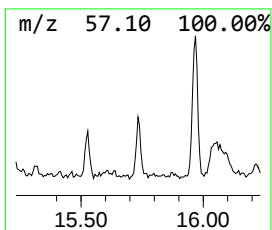
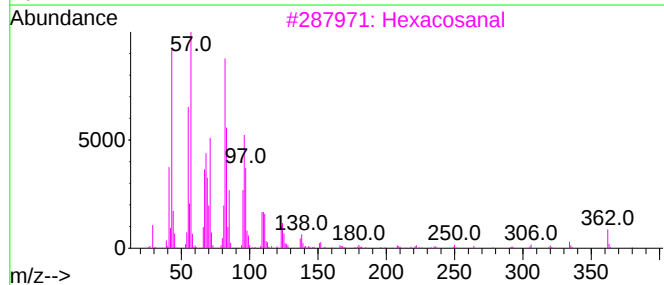
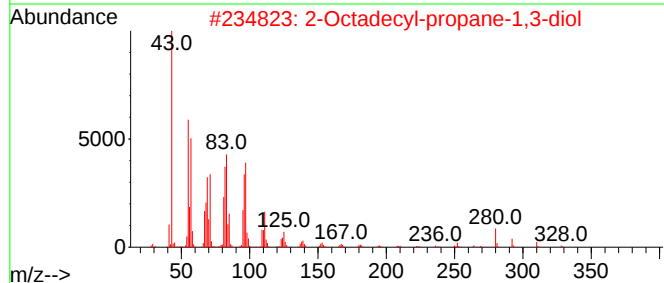
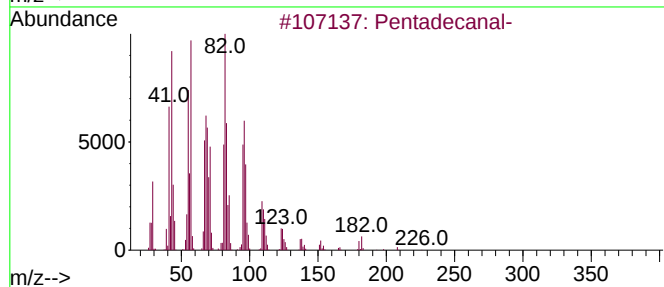
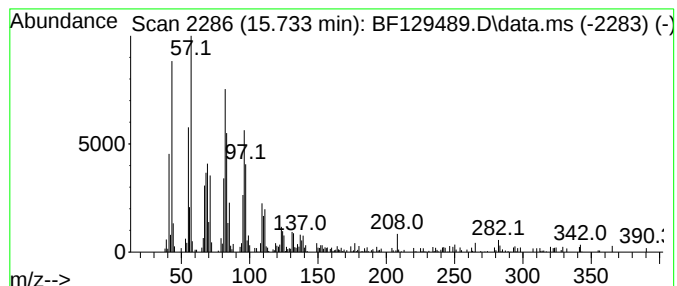
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentadecanal- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	3.28 ng	165808	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanal-	226	C15H30O	002765-11-9	91
2			2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	83
3			Hexacosanal	380	C26H52O	026627-85-0	76
4			Octacosanal	408	C28H56O	022725-64-0	74
5			12-Octadecenal	266	C18H34O	056554-91-7	72



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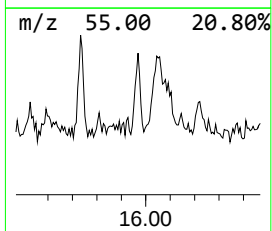
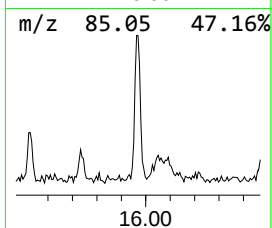
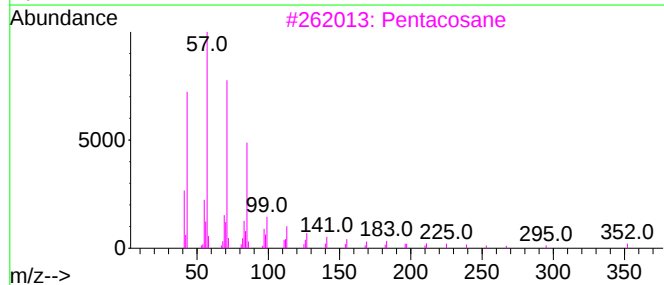
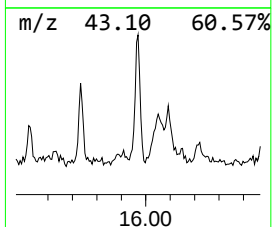
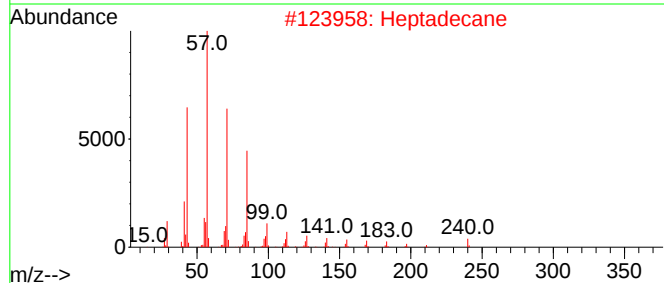
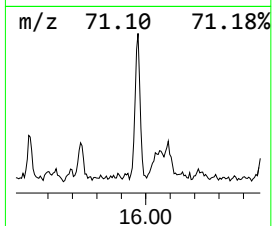
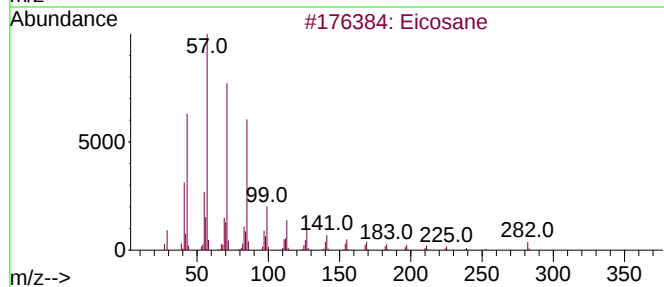
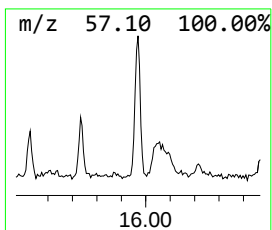
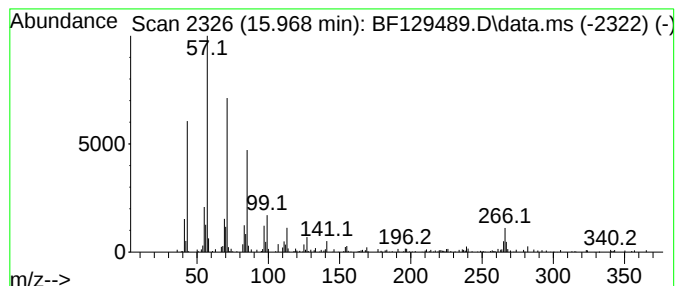
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	3.61 ng	182465	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Heptadecane	240	C17H36	000629-78-7	93
3			Pentacosane	352	C25H52	000629-99-2	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Nonadecane	268	C19H40	000629-92-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129489.D
Acq On : 01 Aug 2022 23:38
Operator : CG\JU
Sample : N3896-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-64

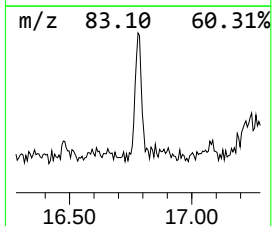
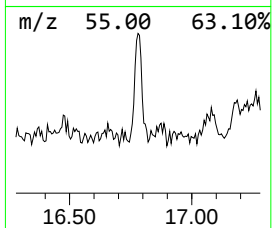
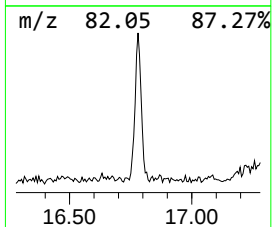
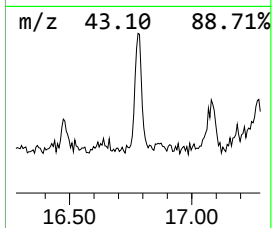
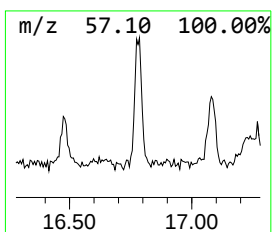
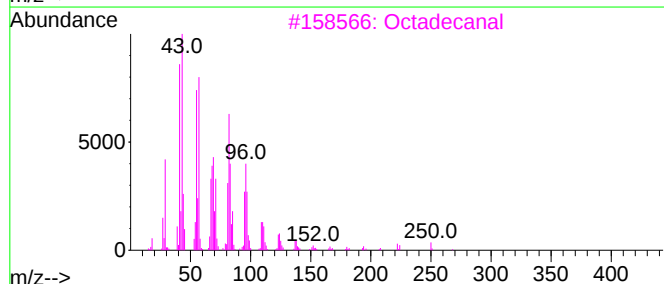
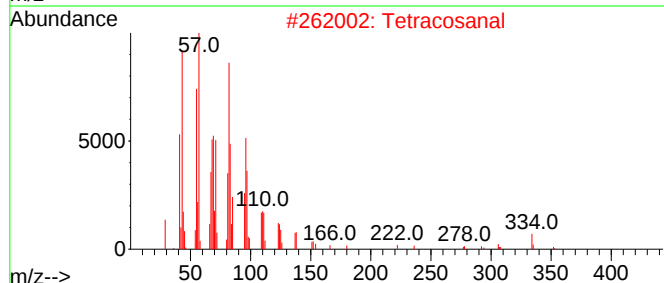
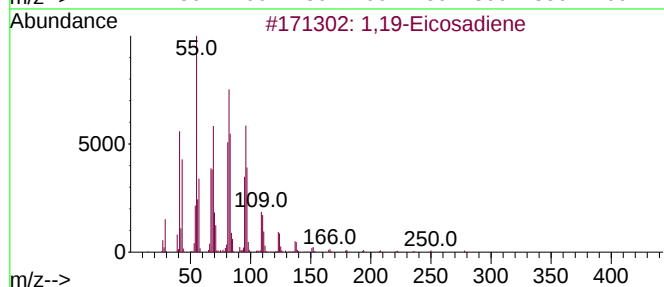
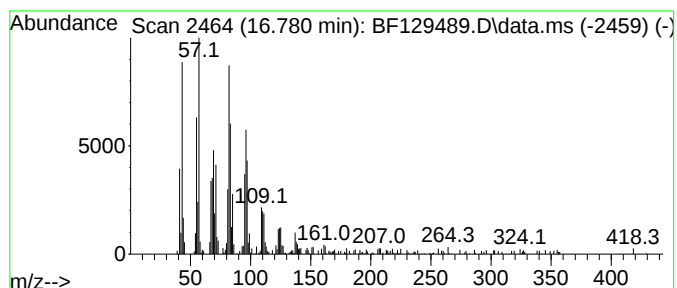
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,19-Eicosadiene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	4.41 ng	222765	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene		278	C20H38	014811-95-1	94
2	Tetracosanal		352	C24H48O	057866-08-7	94
3	Octadecanal		268	C18H36O	000638-66-4	91
4	Triacontanal		436	C30H60O	022725-63-9	91
5	Heptadecanal		254	C17H34O	1000376-70-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129489.D
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Operator : CG\JU
Sample : N3896-07
Misc :
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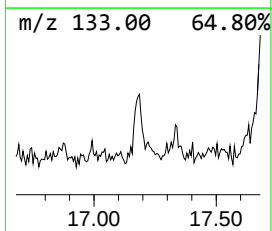
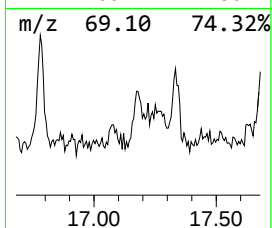
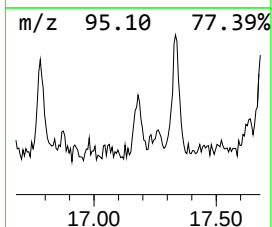
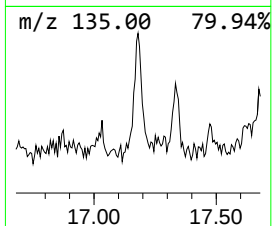
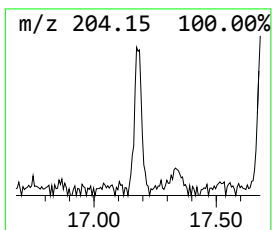
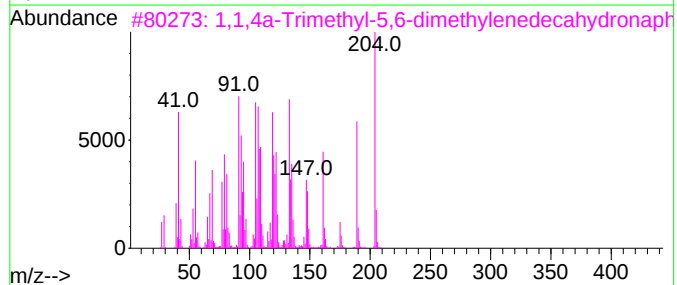
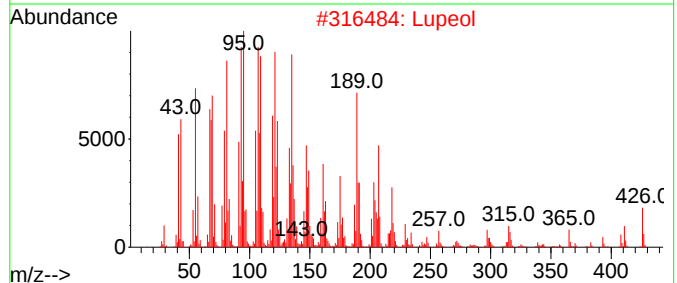
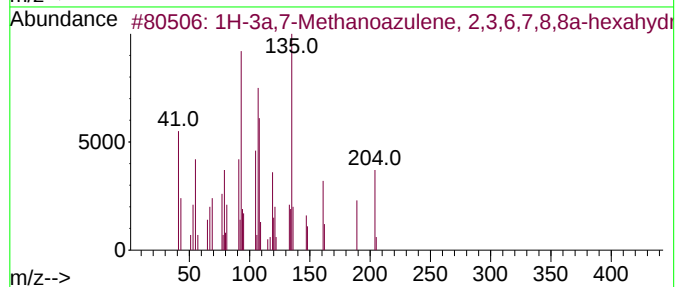
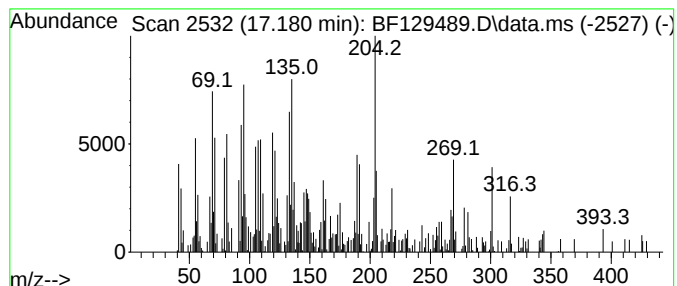
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.180 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.180	5.31 ng	268324	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	46
2	Lupeol	426	C30H50O	000545-47-1	44
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	38
4	(4aS,9aR)-3,5,5,9-Tetramethyl-2,...	204	C15H24	053111-25-4	30
5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129489.D
Acq On : 01 Aug 2022 23:38
Operator : CG\JU
Sample : N3896-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-64

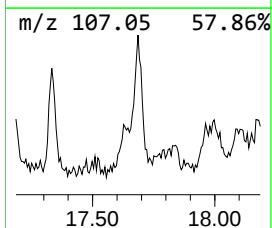
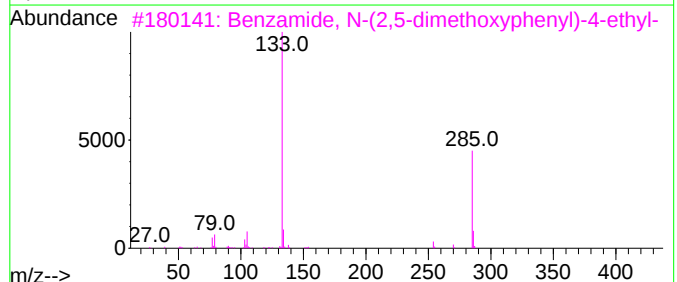
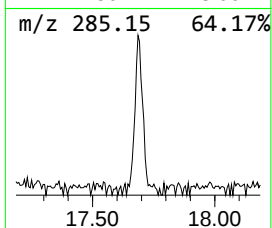
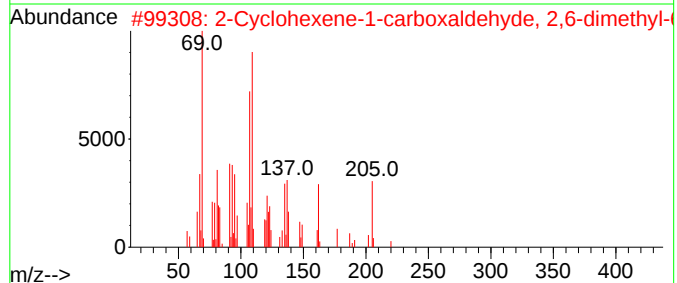
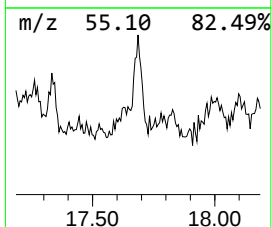
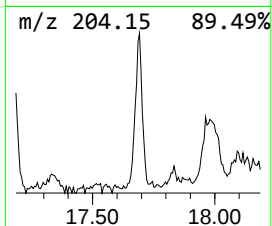
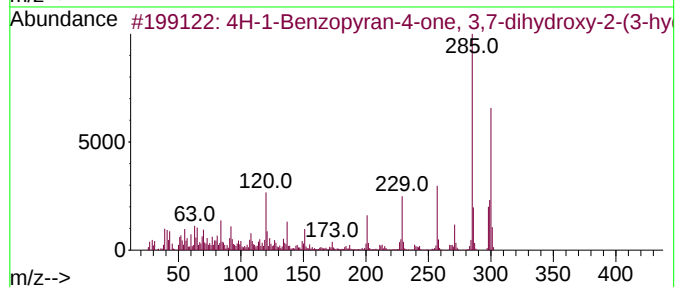
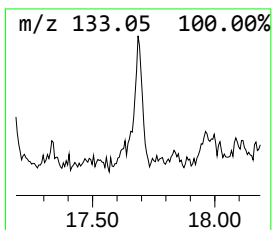
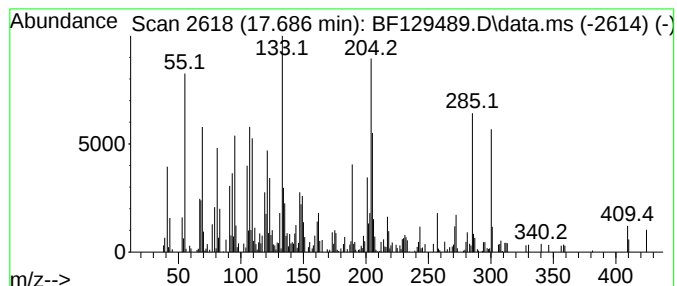
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.686 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.686	6.67 ng	337191	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-1-Benzopyran-4-one, 3,7-dihyd...	300	C16H12O6	057396-72-2	41
2		2-Cyclohexene-1-carboxaldehyde, ...	220	C15H24O	056772-07-7	25
3		Benzamide, N-(2,5-dimethoxypheny...	285	C17H19NO3	1000307-01-8	11
4		4-tert-Butyltoluene	148	C11H16	000098-51-1	11
5		Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129489.D
Acq On : 01 Aug 2022 23:38
Operator : CG\JU
Sample : N3896-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

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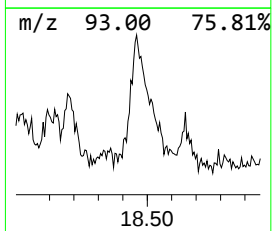
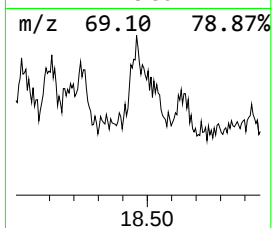
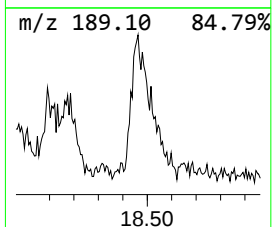
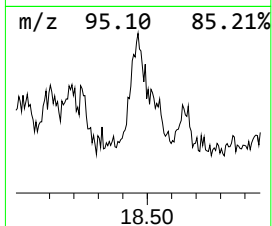
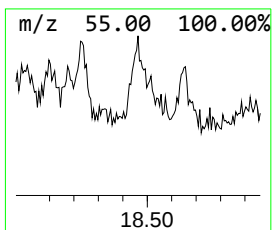
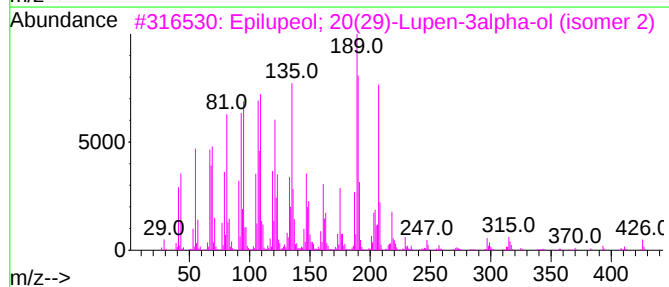
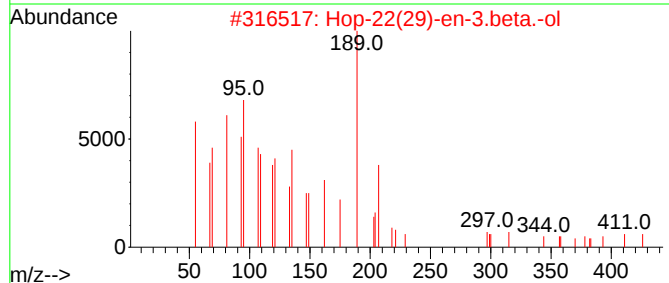
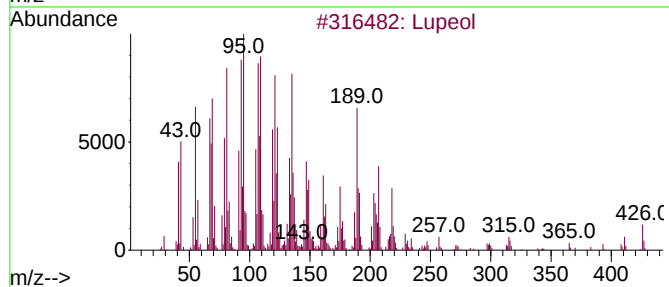
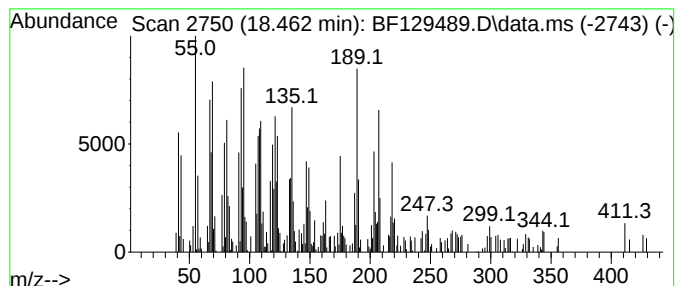
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Lupeol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.462	11.54 ng	583422	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	95
2			Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	89
3			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	64
4			Taraxasterol	426	C30H50O	001059-14-9	43
5			(4aR,11aS)-4a-Methyl-3,4,4a,5,6,...	218	C14H18O2	1000482-61-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080122\
Data File : BF129489.D
Acq On : 01 Aug 2022 23:38
Operator : CG\JU
Sample : N3896-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
5-Eicosene, (E)-	13.874	9.9	ng	568502	5	14.045	1152280	20.0
1-Nonadecene	14.516	11.1	ng	639534	5	14.045	1152280	20.0
Benzo[e]pyrene	15.404	4.0	ng	201107	6	15.527	1011200	20.0
Pentadecanal-	15.733	3.3	ng	165808	6	15.527	1011200	20.0
Eicosane	15.968	3.6	ng	182465	6	15.527	1011200	20.0
1,19-Eicosadiene	16.780	4.4	ng	222765	6	15.527	1011200	20.0
unknown17.180	17.180	5.3	ng	268324	6	15.527	1011200	20.0
unknown17.686	17.686	6.7	ng	337191	6	15.527	1011200	20.0
Lupeol	18.462	11.5	ng	583422	6	15.527	1011200	20.0