

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
 Data File : BF127654.D
 Acq On : 06 Apr 2022 18:12
 Operator : CG\JU
 Sample : N2220-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A04015

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	485	494	498	rVB	47139	63101	2.02%	0.315%
2	5.575	554	559	562	rBV	2315118	2151487	68.81%	10.728%
3	6.575	723	729	732	rBV	2192288	2267852	72.54%	11.308%
4	6.963	791	795	798	rBV	746046	578364	18.50%	2.884%
5	7.522	885	890	893	rBV	1697229	1491319	47.70%	7.436%
6	8.245	1009	1013	1016	rBV	939180	751634	24.04%	3.748%
7	9.322	1192	1196	1200	rBV	2897335	2650137	84.76%	13.214%
8	9.398	1205	1209	1214	rVB	56732	44146	1.41%	0.220%
9	10.004	1309	1312	1316	rVB	991646	889069	28.44%	4.433%
10	10.798	1442	1447	1450	rBV	1990719	1841275	58.89%	9.181%
11	11.498	1562	1566	1570	rBV	1149349	975872	31.21%	4.866%
12	11.886	1629	1632	1635	rVB	61575	43839	1.40%	0.219%
13	12.016	1648	1654	1665	rBV	118152	138303	4.42%	0.690%
14	12.804	1783	1788	1795	rBV	37307	43300	1.38%	0.216%
15	13.092	1832	1837	1840	rBV	3490247	3126536	100.00%	15.590%
16	13.980	1984	1988	1999	rBV	305617	314559	10.06%	1.568%
17	14.145	2009	2016	2020	rBV	1063460	994635	31.81%	4.960%
18	14.245	2028	2033	2041	rBV	401871	471927	15.09%	2.353%
19	15.021	2161	2165	2170	rVB	92759	99913	3.20%	0.498%
20	15.674	2270	2276	2281	rBV2	675867	866900	27.73%	4.323%
21	16.233	2366	2371	2379	rBV3	34107	58211	1.86%	0.290%
22	16.963	2484	2495	2509	rBV3	45460	192604	6.16%	0.960%

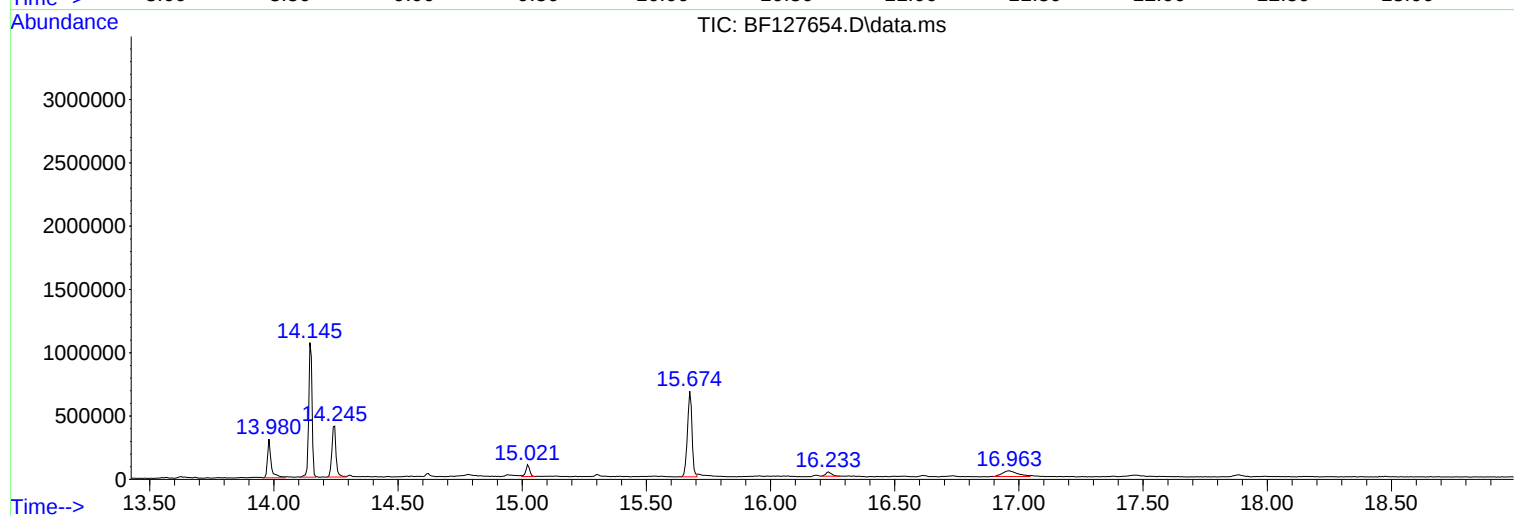
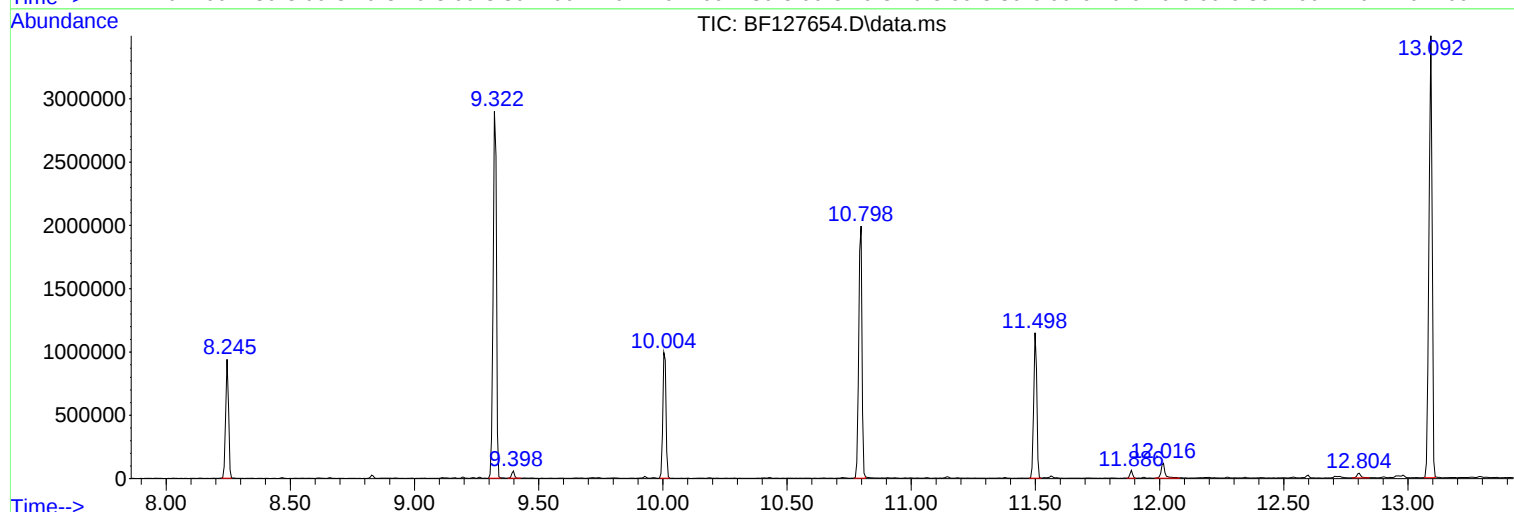
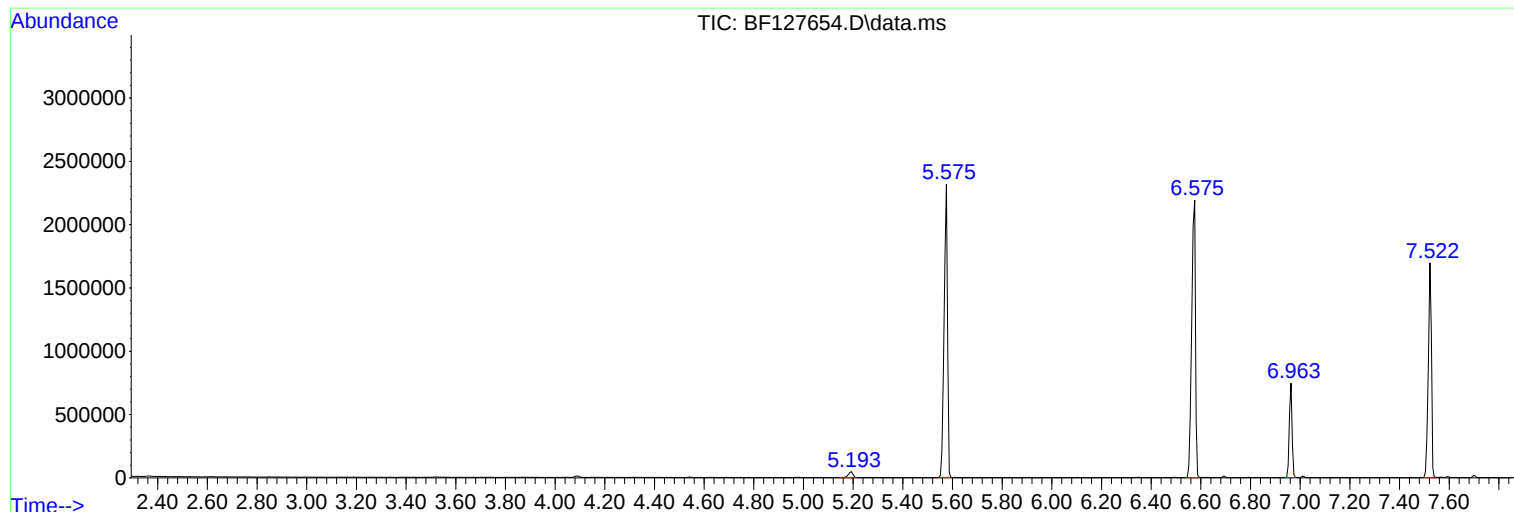
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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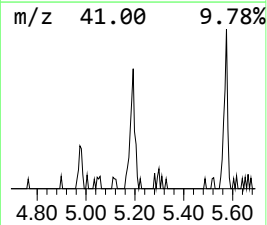
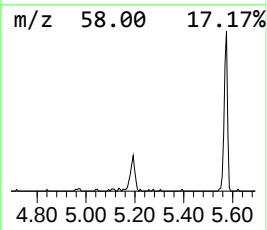
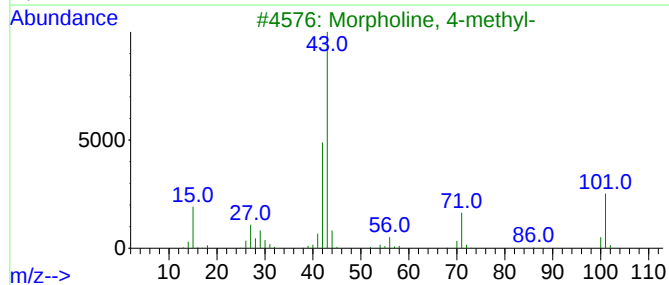
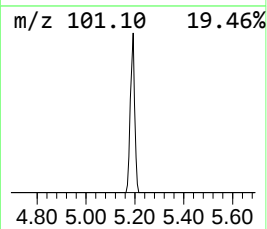
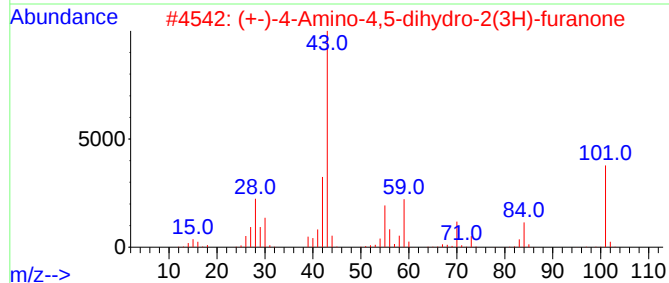
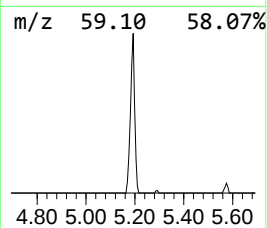
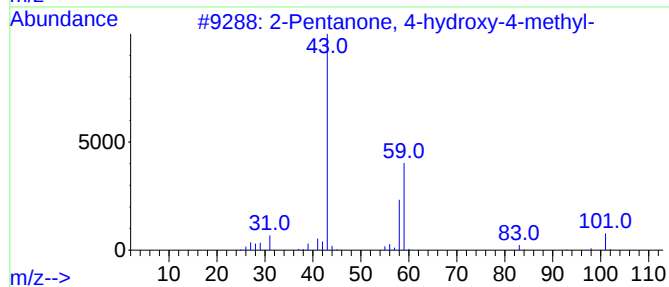
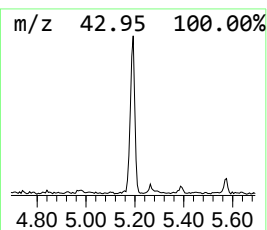
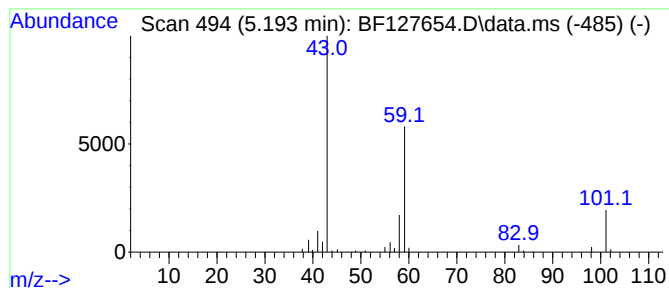
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.193	2.18 ng	63101	1,4-Dichlorobenzene-d4		6.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9
3	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	9



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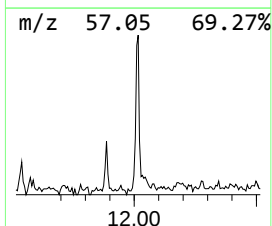
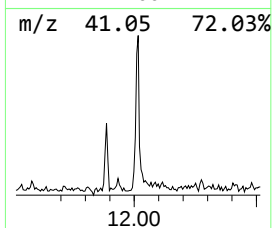
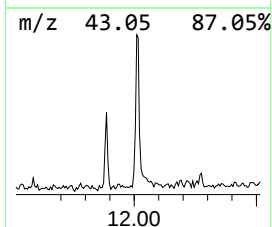
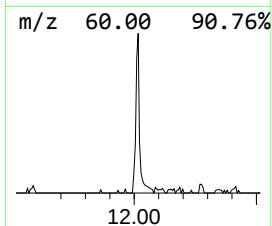
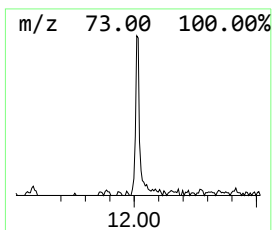
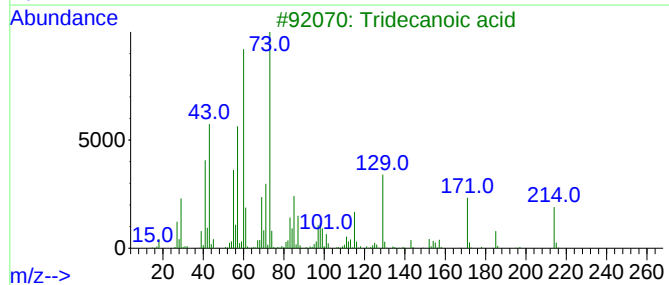
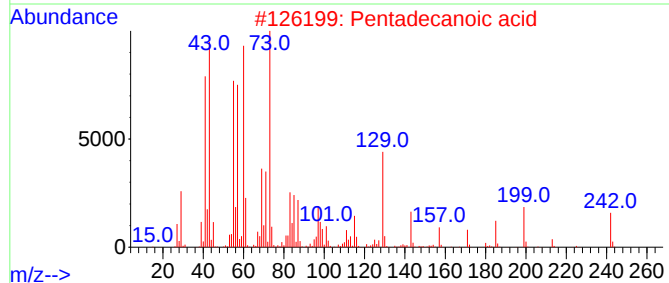
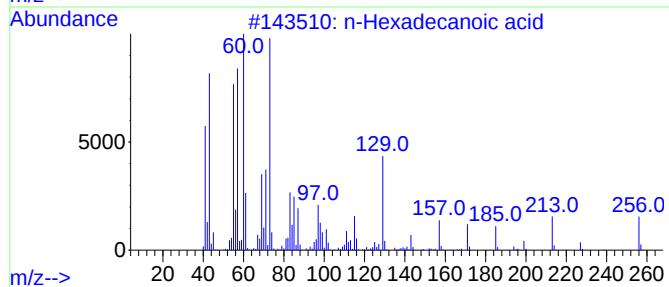
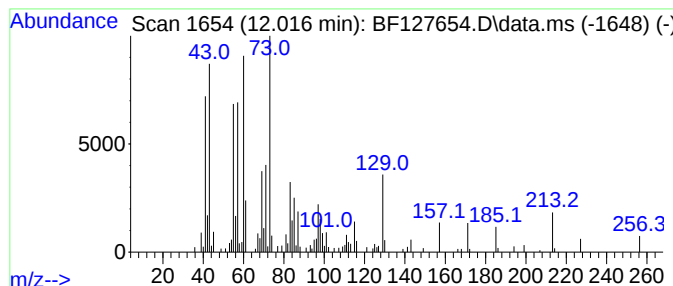
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	2.83 ng	138303	Phenanthrene-d10	11.498

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	68
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	30
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	20



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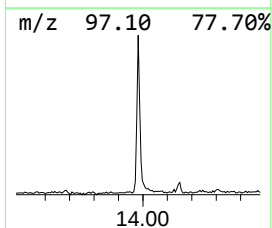
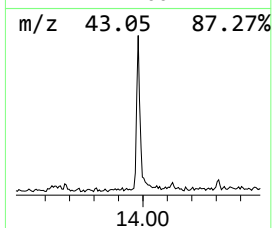
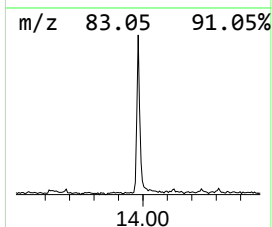
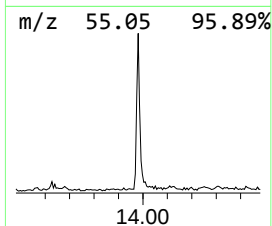
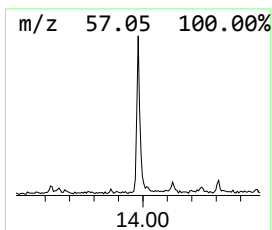
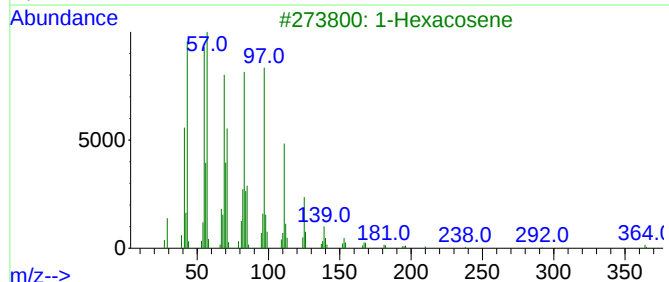
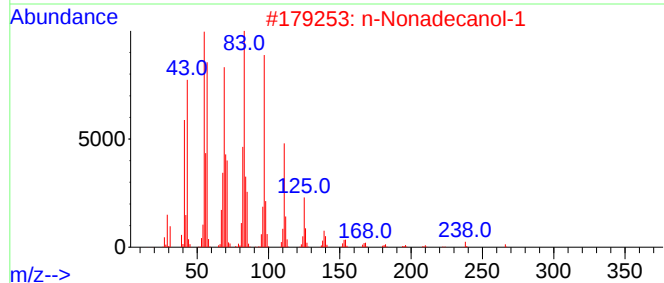
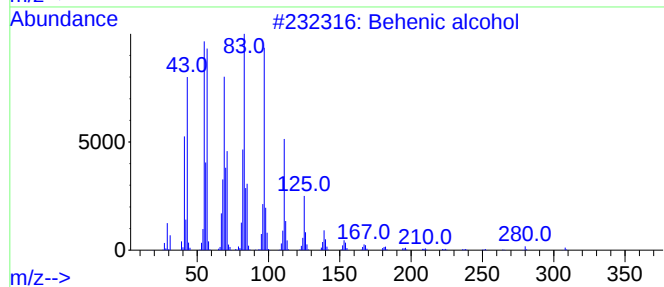
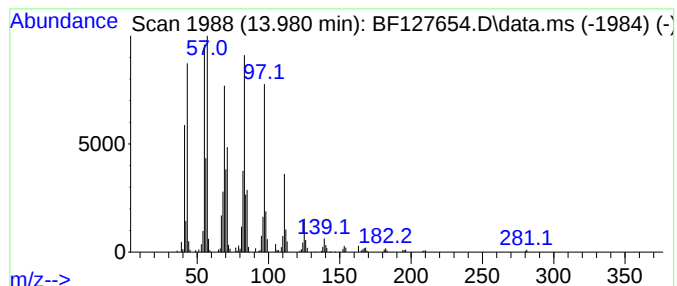
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Peak Number 3 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	6.33 ng	314559	Chrysene-d12	14.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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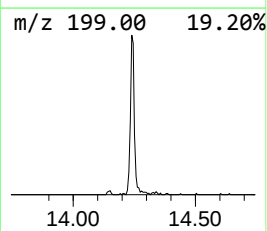
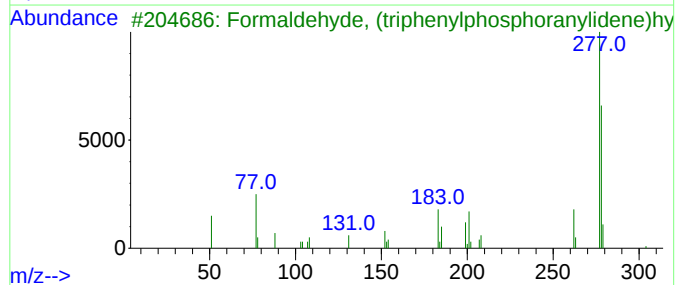
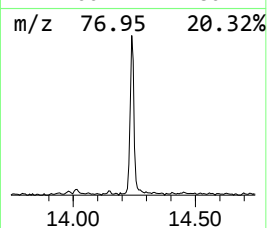
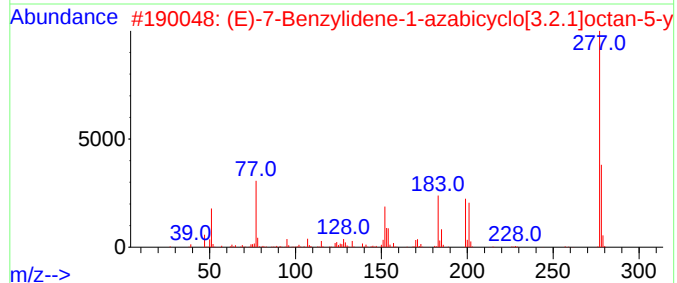
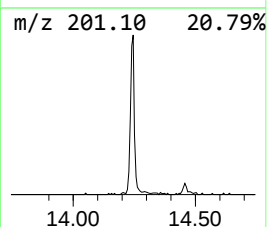
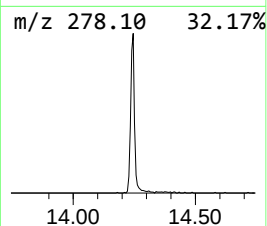
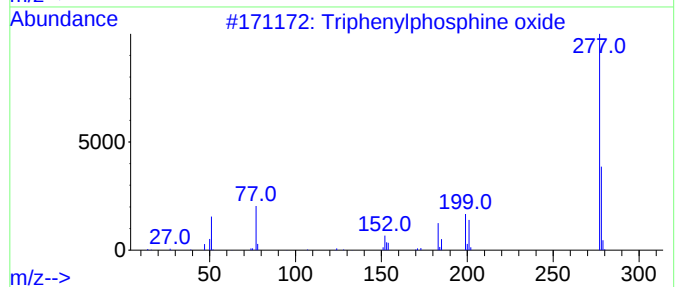
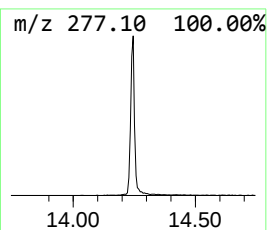
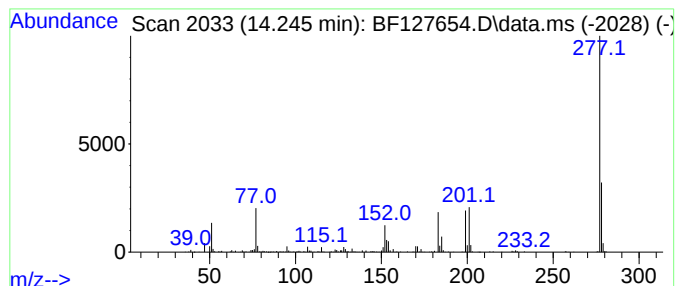
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	9.49 ng	471927	Chrysene-d12	14.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	40
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	9
5			5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	9



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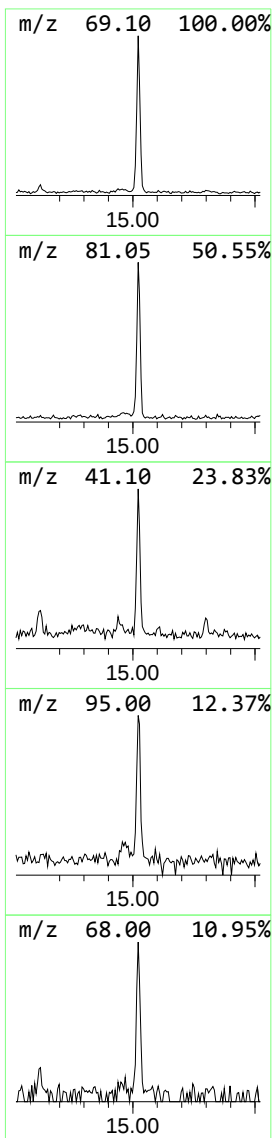
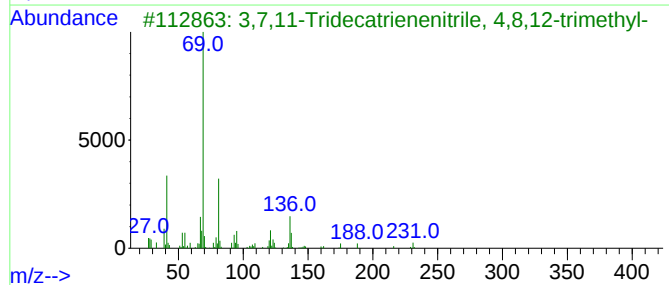
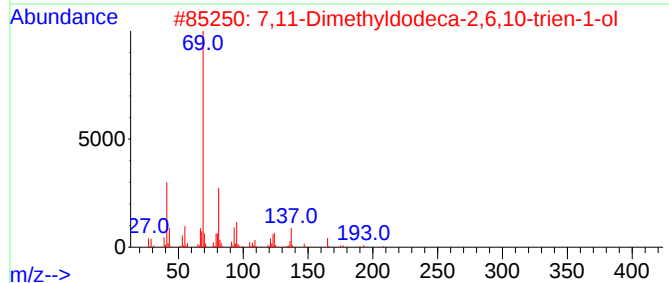
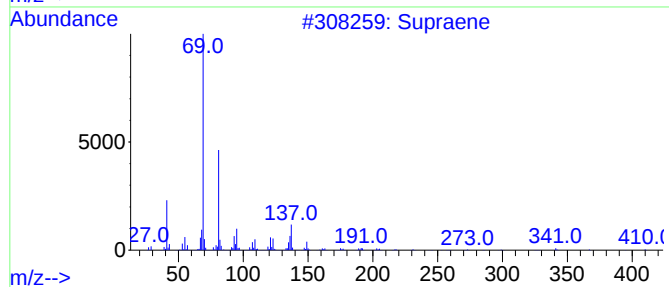
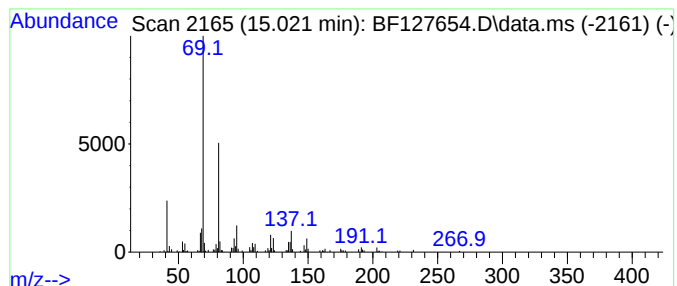
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.022	2.31 ng	99913	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
3			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
4			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



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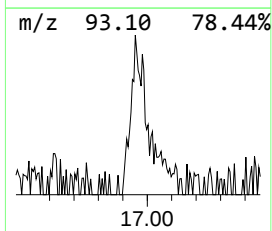
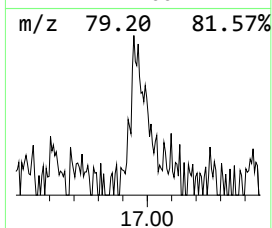
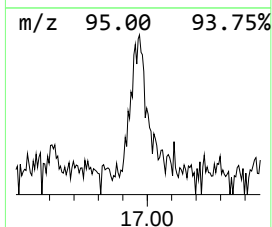
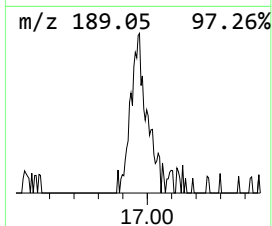
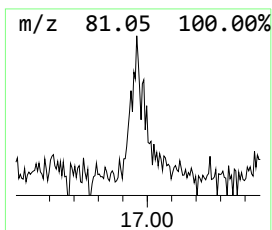
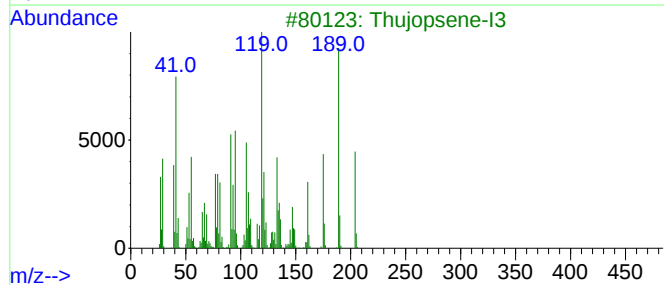
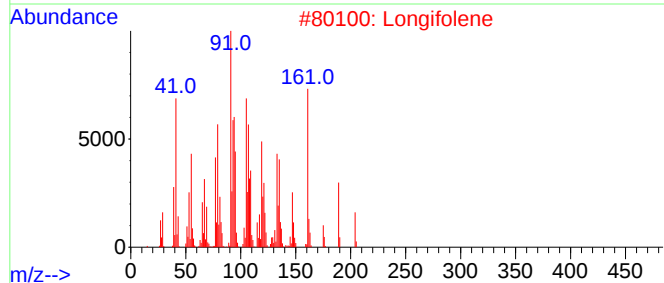
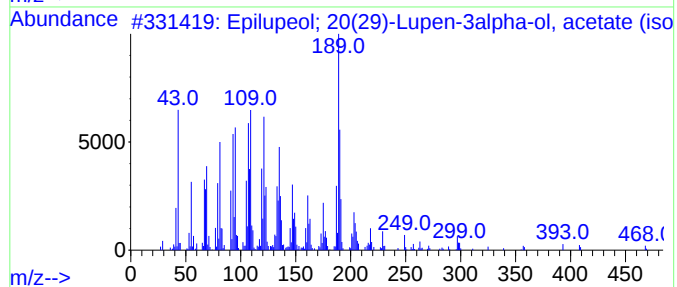
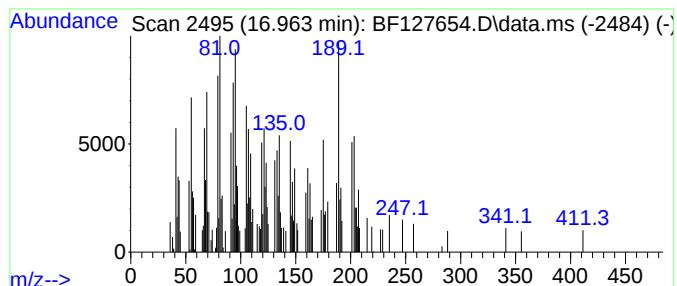
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.962 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.962	4.44 ng	192604	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	49
2			Longifolene	204	C15H24	000475-20-7	41
3			Thujopsene-I3	204	C15H24	1000162-77-8	35
4			Ethanone, 1-[4-(trifluoromethoxy...	204	C9H7F3O2	085013-98-5	35
5			Dimethyl(bis[(4,8,8-trimethyldec...	500	C32H56O2Si	1000364-69-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040622\
Data File : BF127654.D
Acq On : 06 Apr 2022 18:12
Operator : CG\JU
Sample : N2220-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A04015

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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-Pentanone, 4-...	5.193	2.2	ng	63101	1	6.963	578364	20.0
n-Hexadecanoic ...	12.016	2.8	ng	138303	4	11.498	975872	20.0
Behenic alcohol	13.980	6.3	ng	314559	5	14.145	994635	20.0
Triphenylphosph...	14.245	9.5	ng	471927	5	14.145	994635	20.0
Supraene	15.022	2.3	ng	99913	6	15.674	866900	20.0
unknown16.962	16.962	4.4	ng	192604	6	15.674	866900	20.0