

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032222\
 Data File : BF127454.D
 Acq On : 22 Mar 2022 16:22
 Operator : CG\JU
 Sample : N1996-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FT-TOTTEN-MW-01-GW

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-BF032122.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127454.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	538	541	557	rBV	975531	956708	25.94%	5.086%
2	6.475	709	712	730	rBV	548130	604309	16.39%	3.212%
3	6.846	771	775	782	rBV	752545	630722	17.10%	3.353%
4	7.416	867	872	875	rBV	2198665	2176375	59.02%	11.569%
5	8.128	989	993	1000	rBV	1012069	857247	23.25%	4.557%
6	9.204	1171	1176	1179	rBV	3901000	3685871	99.95%	19.593%
7	9.886	1288	1292	1295	rBV	1089001	1019725	27.65%	5.421%
8	10.675	1422	1426	1430	rBV	1743633	1724461	46.76%	9.167%
9	11.375	1542	1545	1549	rBV	1352083	1092995	29.64%	5.810%
10	12.469	1725	1731	1740	rVB2	39071	87998	2.39%	0.468%
11	12.963	1810	1815	1818	rBV	3622599	3687685	100.00%	19.602%
12	13.316	1868	1875	1882	rBV	55720	105348	2.86%	0.560%
13	13.957	1977	1984	1987	rBV2	91180	151416	4.11%	0.805%
14	14.022	1992	1995	2011	rVB	835753	786094	21.32%	4.179%
15	14.480	2067	2073	2077	rBV	71401	106242	2.88%	0.565%
16	14.969	2152	2156	2162	rVB	62280	90171	2.45%	0.479%
17	15.033	2162	2167	2174	rBV4	67405	113226	3.07%	0.602%
18	15.504	2242	2247	2260	rBV	466639	668811	18.14%	3.555%
19	16.163	2353	2359	2364	rBV2	27680	58757	1.59%	0.312%
20	16.774	2456	2463	2464	rBV7	26219	51203	1.39%	0.272%
21	17.157	2524	2528	2539	rVB8	36463	96330	2.61%	0.512%
22	17.327	2553	2557	2565	rVB8	24344	60684	1.65%	0.323%

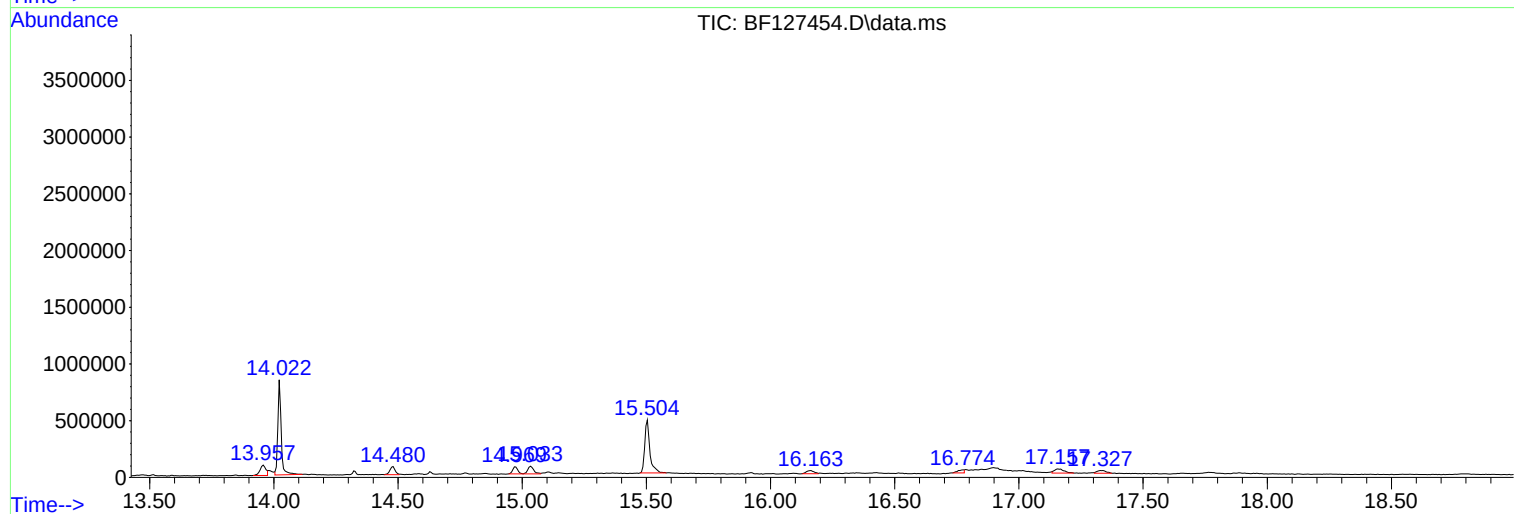
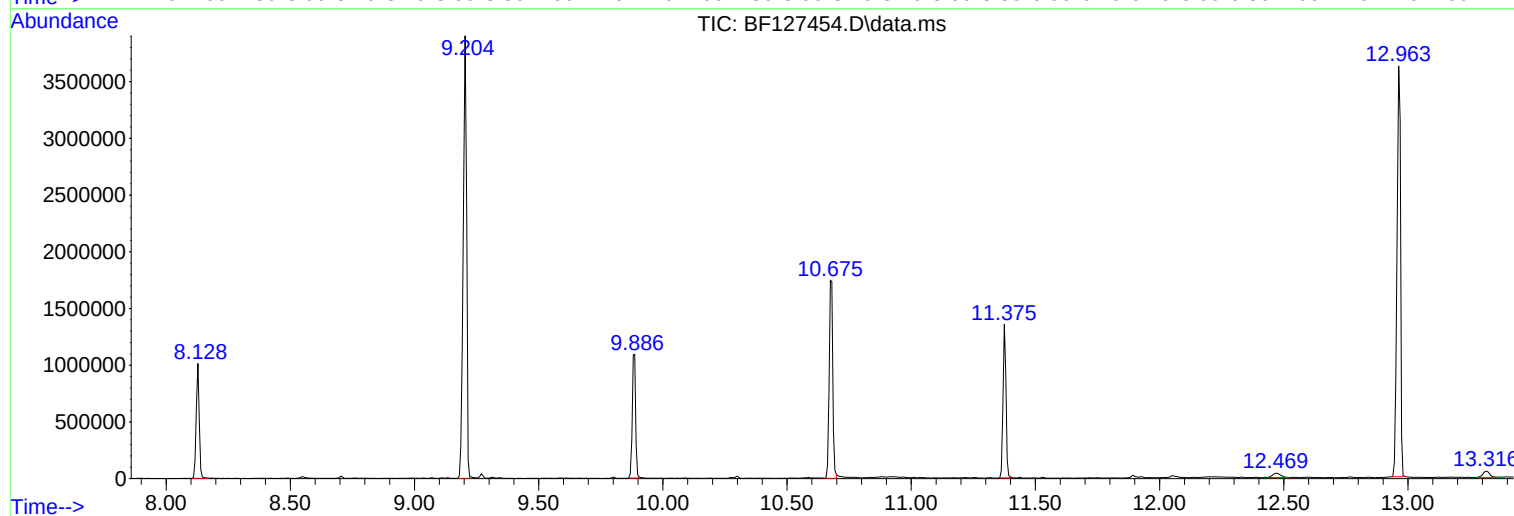
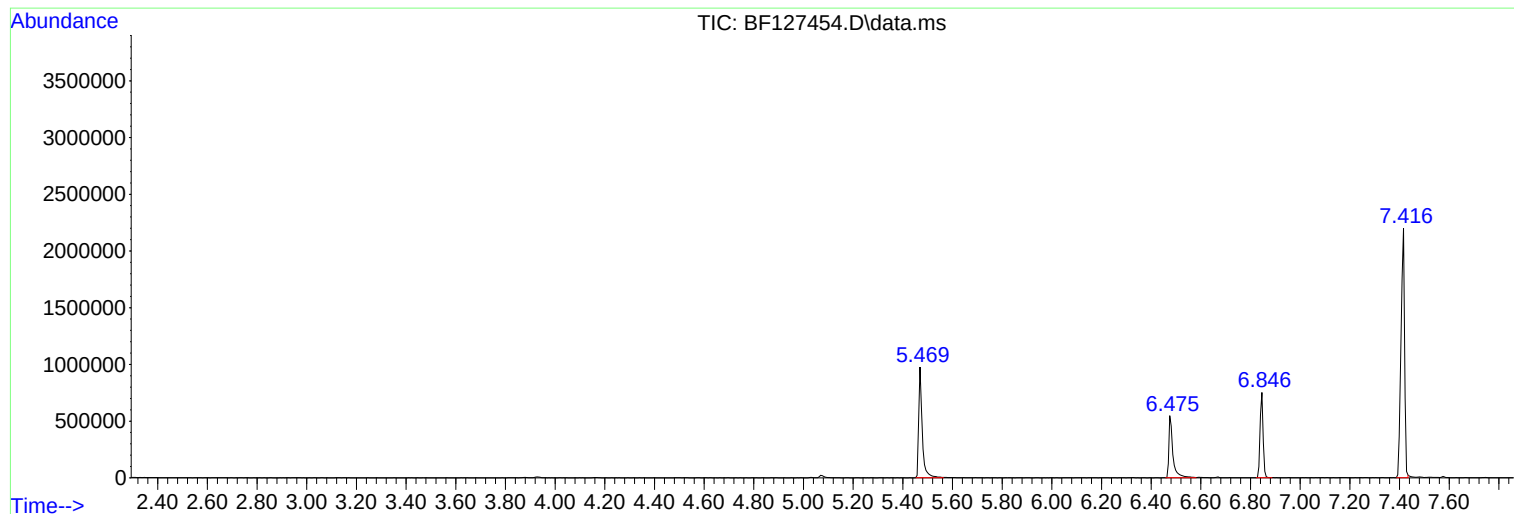
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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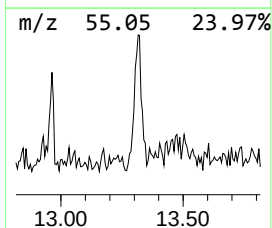
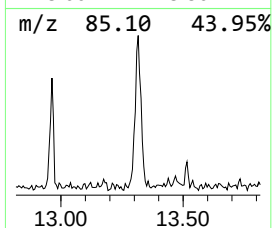
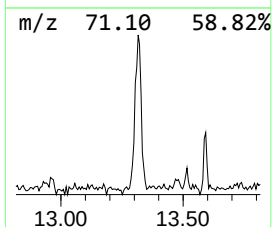
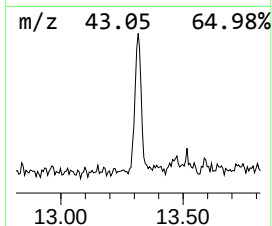
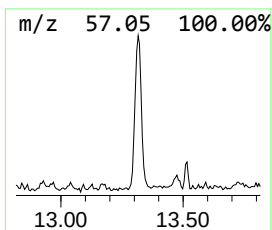
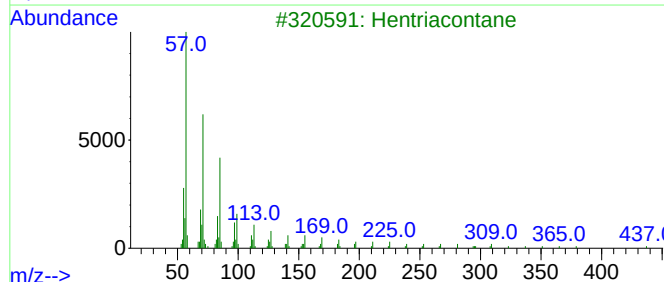
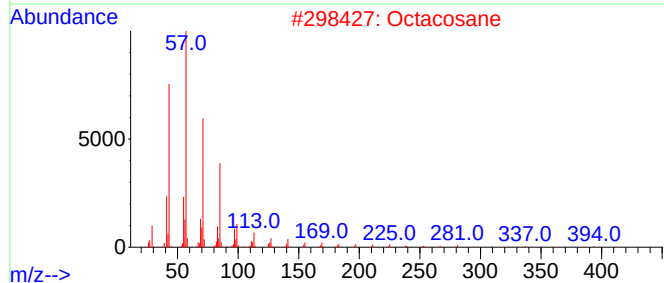
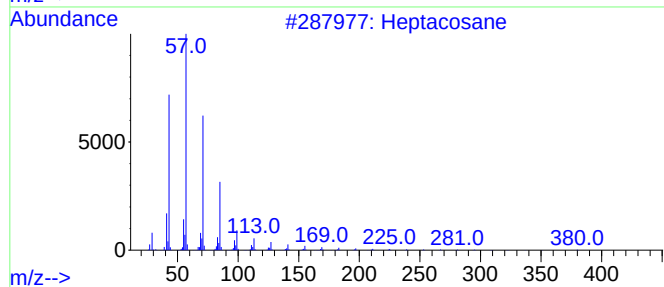
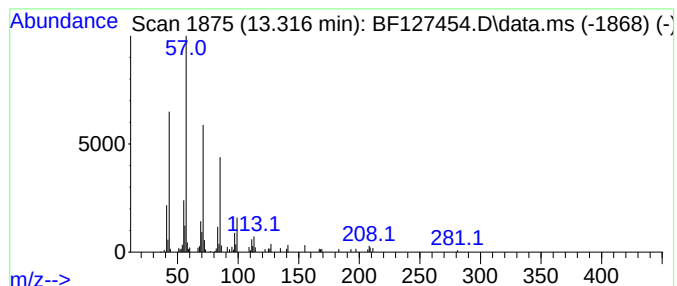
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.316	2.68 ng	105348	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Hentriacontane	437	C31H64	000630-04-6	86
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80



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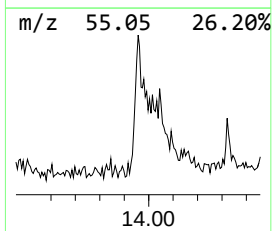
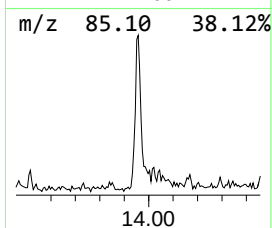
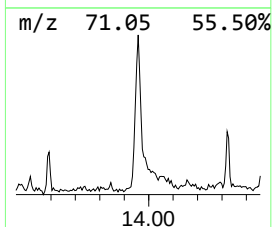
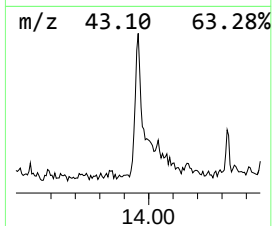
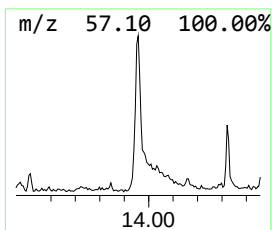
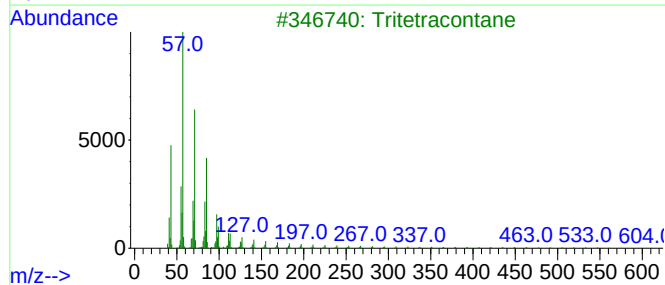
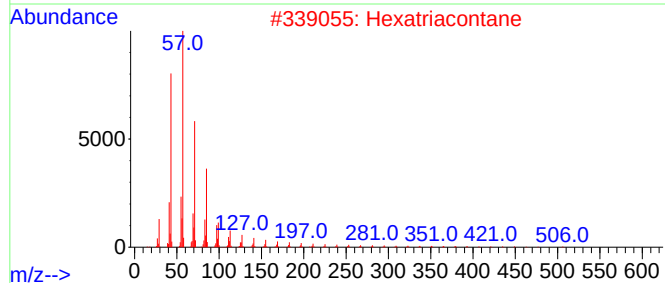
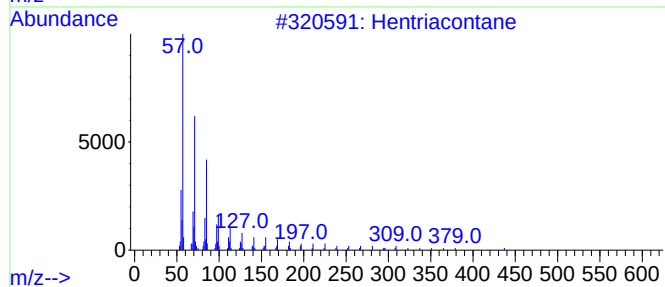
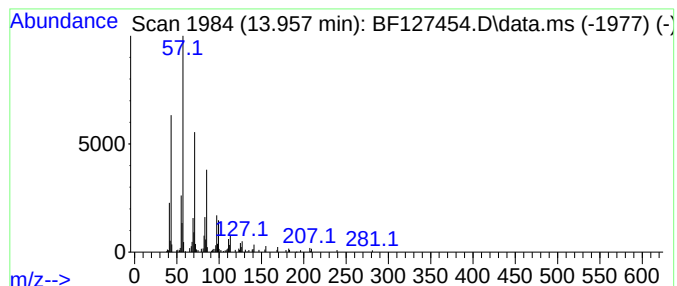
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hentriacontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	3.85 ng	151416	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Hexatriacontane	507	C36H74	000630-06-8	91
3			Tritetracontane	605	C43H88	007098-21-7	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Heneicosane	296	C21H44	000629-94-7	90



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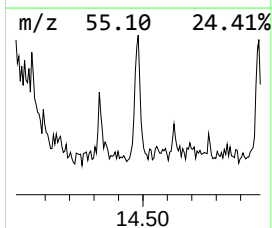
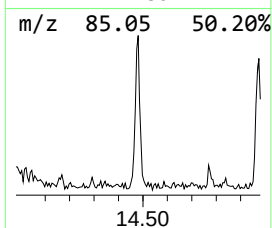
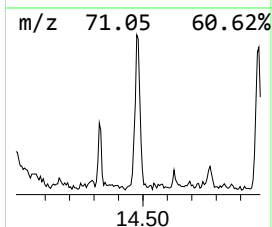
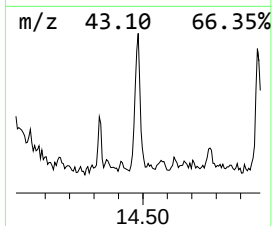
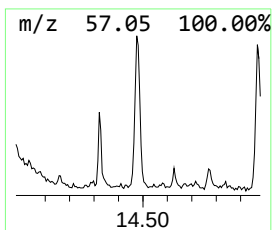
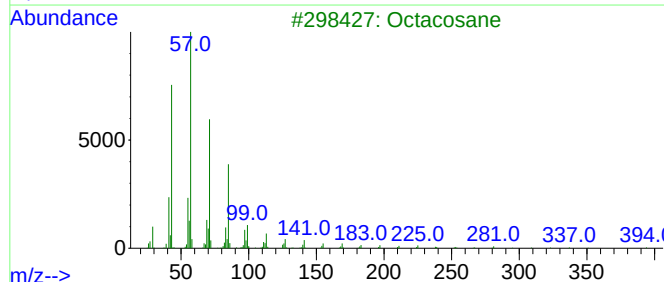
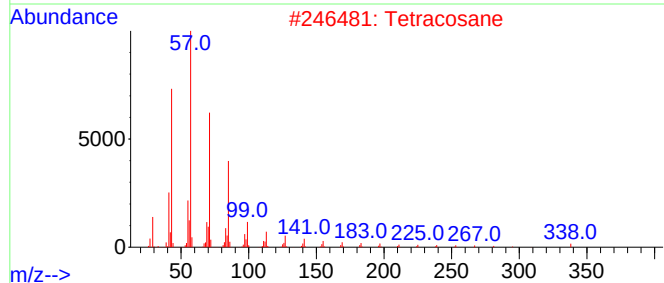
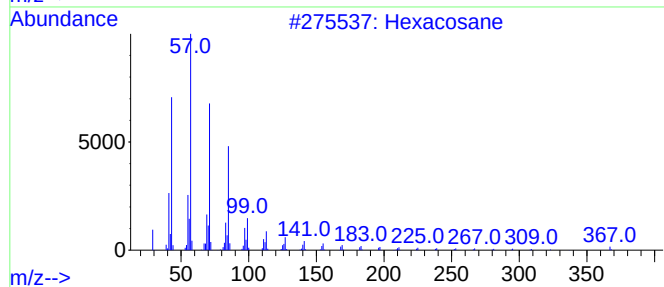
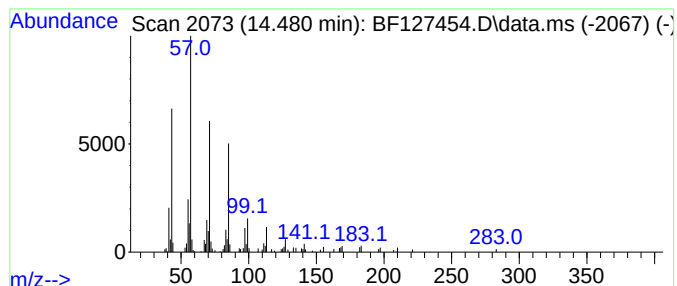
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	2.70 ng	106242	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5			Heneicosane	296	C21H44	000629-94-7	90



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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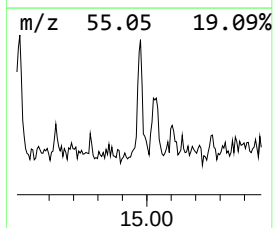
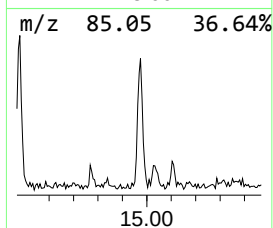
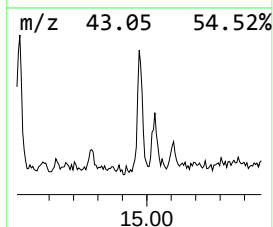
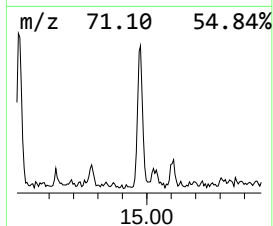
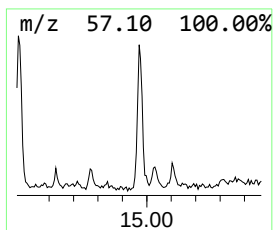
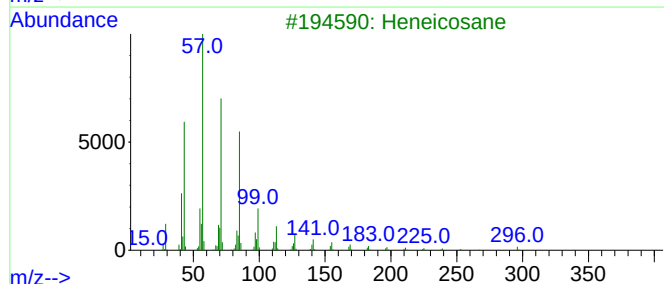
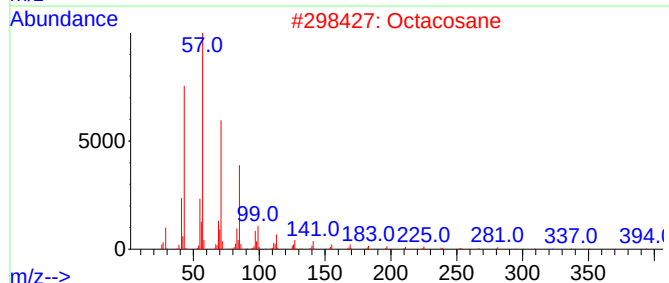
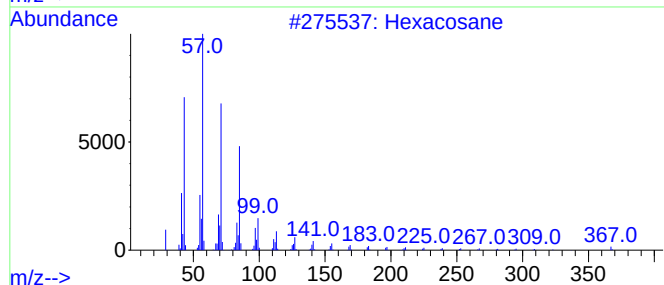
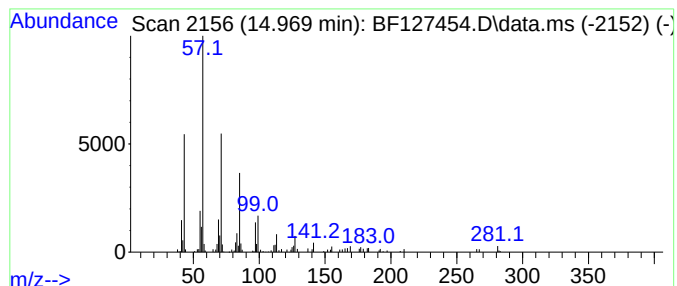
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.969	2.70 ng	90171	Perylene-d12	15.504

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Heneicosane	296	C21H44	000629-94-7	83
4		Heptadecane	240	C17H36	000629-78-7	80
5		Heptacosane	380	C27H56	000593-49-7	80



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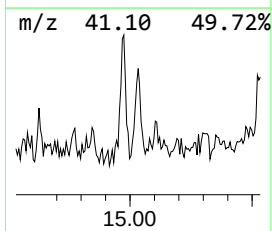
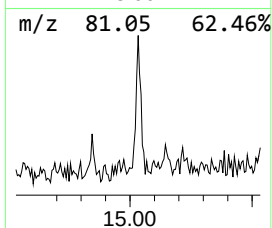
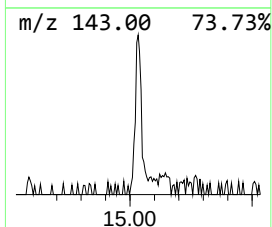
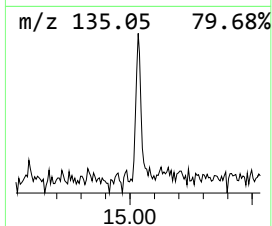
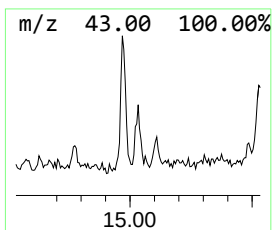
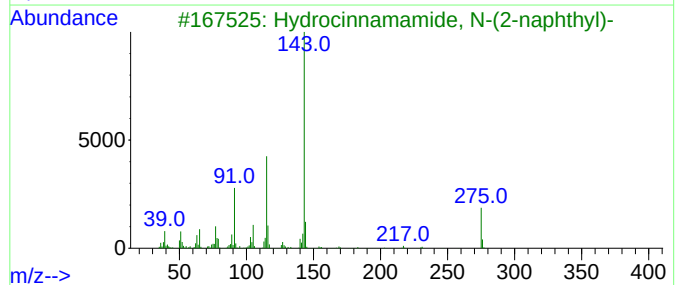
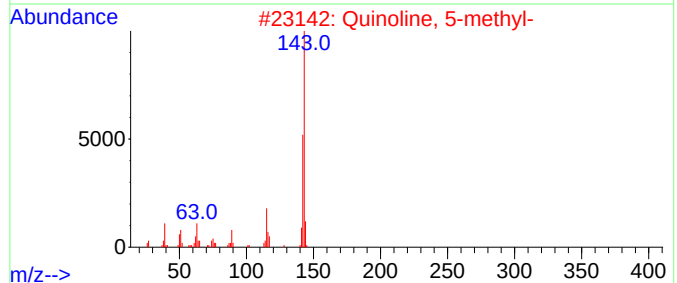
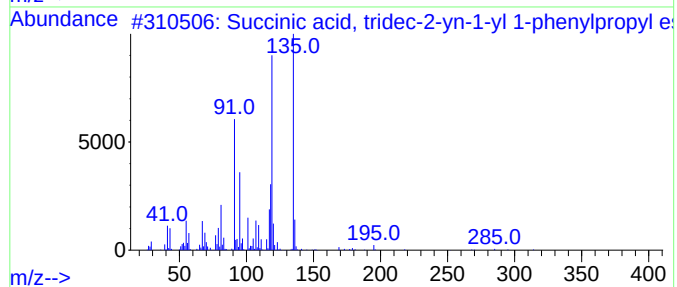
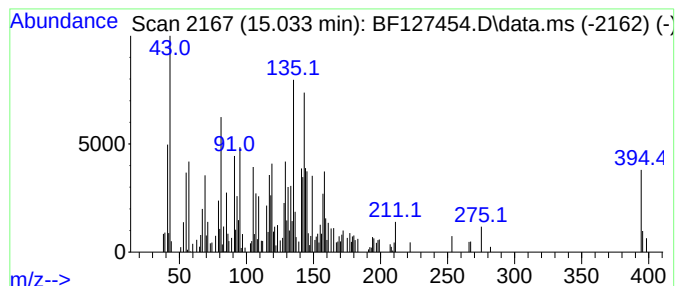
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.033 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	3.39 ng	113226	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, tridec-2-yn-1-yl ...	414	C26H38O4	1000389-93-7	22
2			Quinoline, 5-methyl-	143	C10H9N	007661-55-4	11
3			Hydrocinnamamide, N-(2-naphthyl)-	275	C19H17NO	055685-46-6	11
4			1-Adamantyl methyl ketone	178	C12H18O	001660-04-4	10
5			2,4-Methano-1H-indene, 4-chloroo...	170	C10H15Cl	098640-25-6	10



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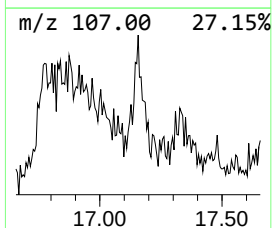
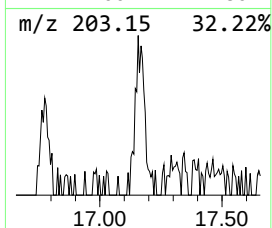
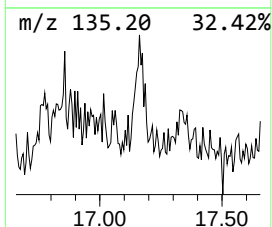
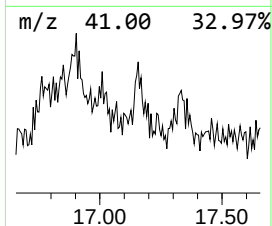
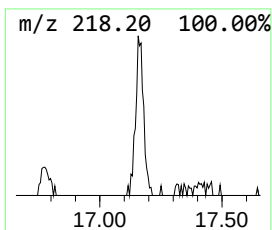
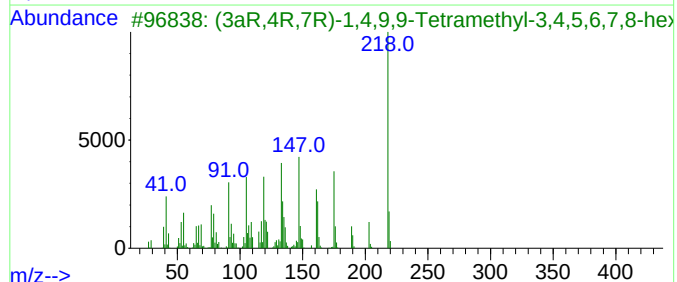
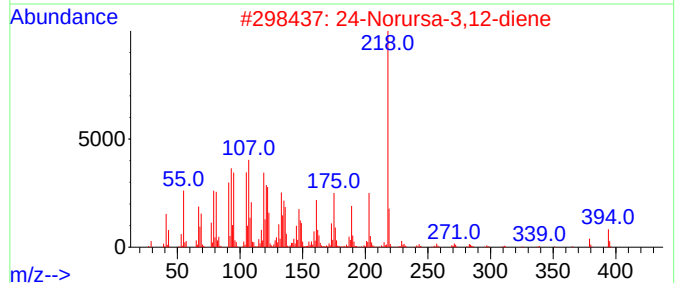
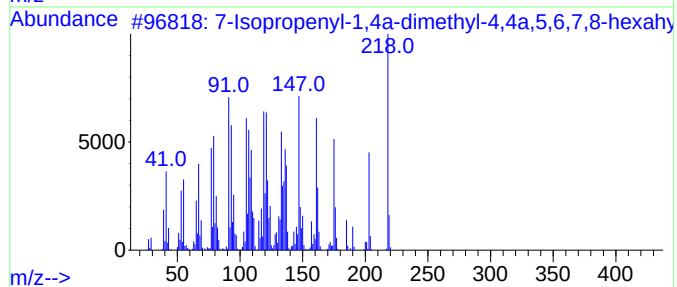
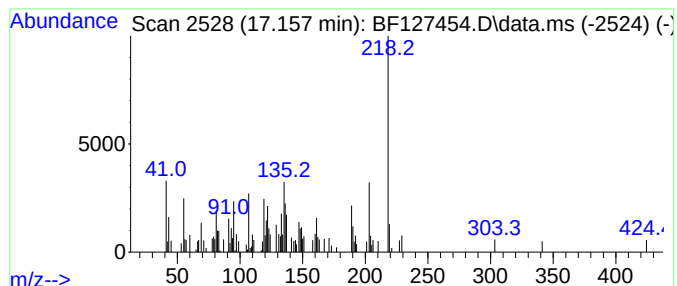
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 7-Isopropenyl-1,4a-dimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.157	2.88 ng	96330	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Isopropenyl-1,4a-dimethyl-4,4a...	218	C15H22O	000473-08-5	83		
2	24-Norursa-3,12-diene	394	C29H46	201358-25-0	64		
3	(3aR,4R,7R)-1,4,9,9-Tetramethyl...	218	C15H22O	003466-15-7	41		
4	1H-Pyrrolo[3,4-c]quinoline-1,3,4...	218	C11H10N2O3	181021-85-2	41		
5	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032222\
Data File : BF127454.D
Acq On : 22 Mar 2022 16:22
Operator : CG\JU
Sample : N1996-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FT-TOTTEN-MW-01-GW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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
Heptacosane	13.316	2.7	ng	105348	5	14.022	786094	20.0
Hentriacontane	13.957	3.9	ng	151416	5	14.022	786094	20.0
Hexacosane	14.480	2.7	ng	106242	5	14.022	786094	20.0
Octacosane	14.969	2.7	ng	90171	6	15.504	668811	20.0
unknown15.033	15.033	3.4	ng	113226	6	15.504	668811	20.0
7-Isopropenyl-1...	17.157	2.9	ng	96330	6	15.504	668811	20.0