

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
 Data File : BF133224.D
 Acq On : 04 May 2023 11:07
 Operator : CG\JU
 Sample : PB152560BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB152560BL

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	11	rVB	171256	202877	2.77%	0.374%
2	4.940	478	485	498	rVB	2332148	3521591	48.17%	6.493%
3	5.351	550	555	558	rBV	5518607	6598013	90.25%	12.166%
4	6.375	722	729	731	rBV	5301748	6607407	90.38%	12.183%
5	6.728	785	789	792	rBV	1816846	1509473	20.65%	2.783%
6	7.298	879	886	888	rBV	3855642	4437545	60.70%	8.182%
7	8.010	1002	1007	1010	rBV	2721614	2155485	29.48%	3.974%
8	9.092	1184	1191	1194	rBV	7037855	7055787	96.51%	13.010%
9	9.763	1297	1305	1308	rBV	3096871	2520789	34.48%	4.648%
10	10.557	1433	1440	1443	rBV	4043857	4421892	60.48%	8.153%
11	11.245	1553	1557	1560	rBV	3087580	2573759	35.20%	4.746%
12	12.839	1822	1828	1831	rBV	6549357	7310883	100.00%	13.480%
13	13.363	1914	1917	1923	rBV	91381	81602	1.12%	0.150%
14	13.880	2000	2005	2008	rBV	2188366	2059886	28.18%	3.798%
15	14.362	2080	2087	2091	rBV	120468	133138	1.82%	0.245%
16	14.657	2131	2137	2142	rBV	159614	179063	2.45%	0.330%
17	14.980	2188	2192	2198	rVB	185313	197152	2.70%	0.364%
18	15.298	2240	2246	2250	rBV	1481027	1683069	23.02%	3.103%
19	15.339	2250	2253	2262	rVB	170480	225521	3.08%	0.416%
20	15.751	2318	2323	2328	rVB	126855	179303	2.45%	0.331%
21	16.227	2398	2404	2408	rBV3	141928	313878	4.29%	0.579%
22	16.780	2492	2498	2507	rVB2	76826	148518	2.03%	0.274%
23	17.439	2603	2610	2617	rVB2	52021	117957	1.61%	0.217%

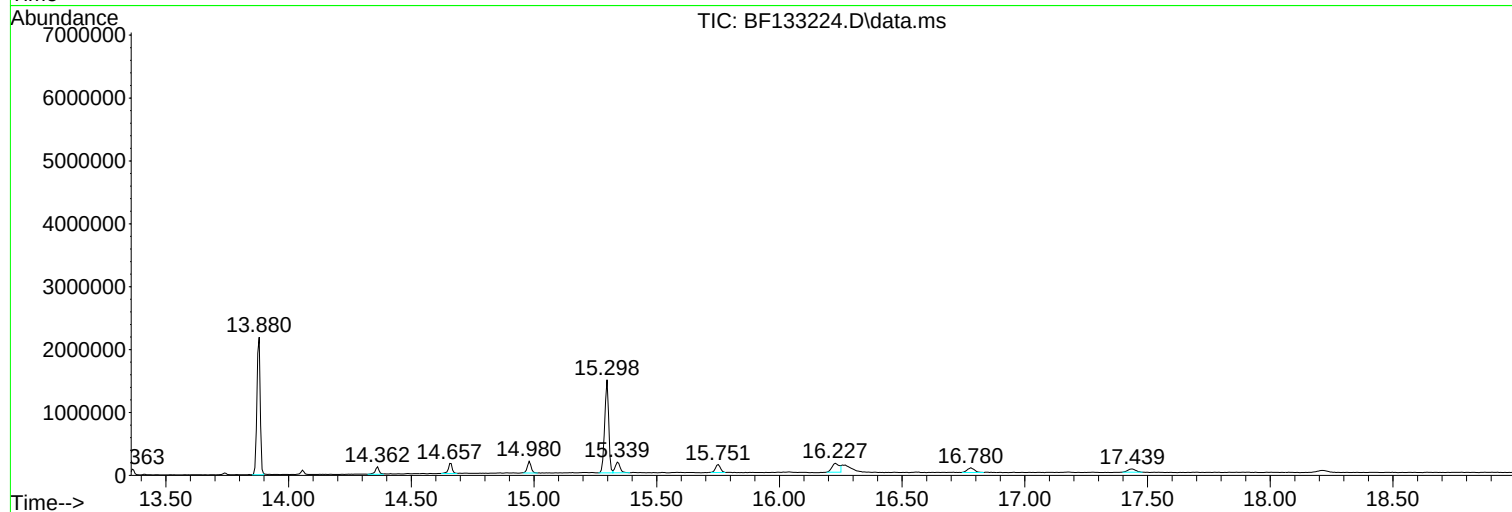
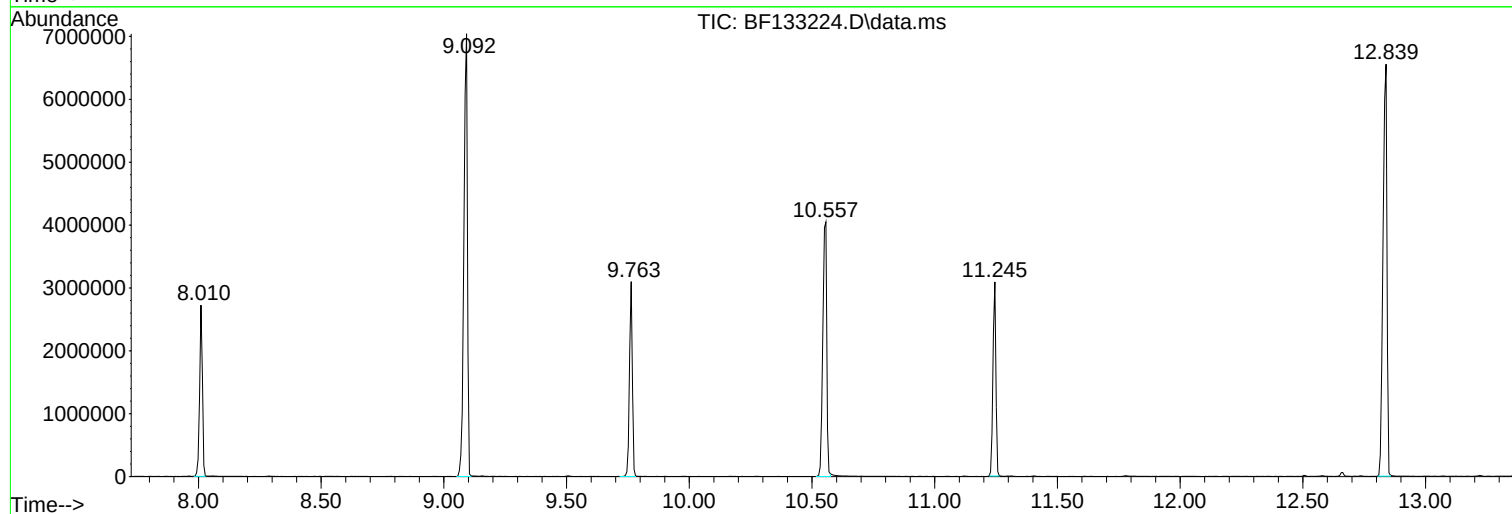
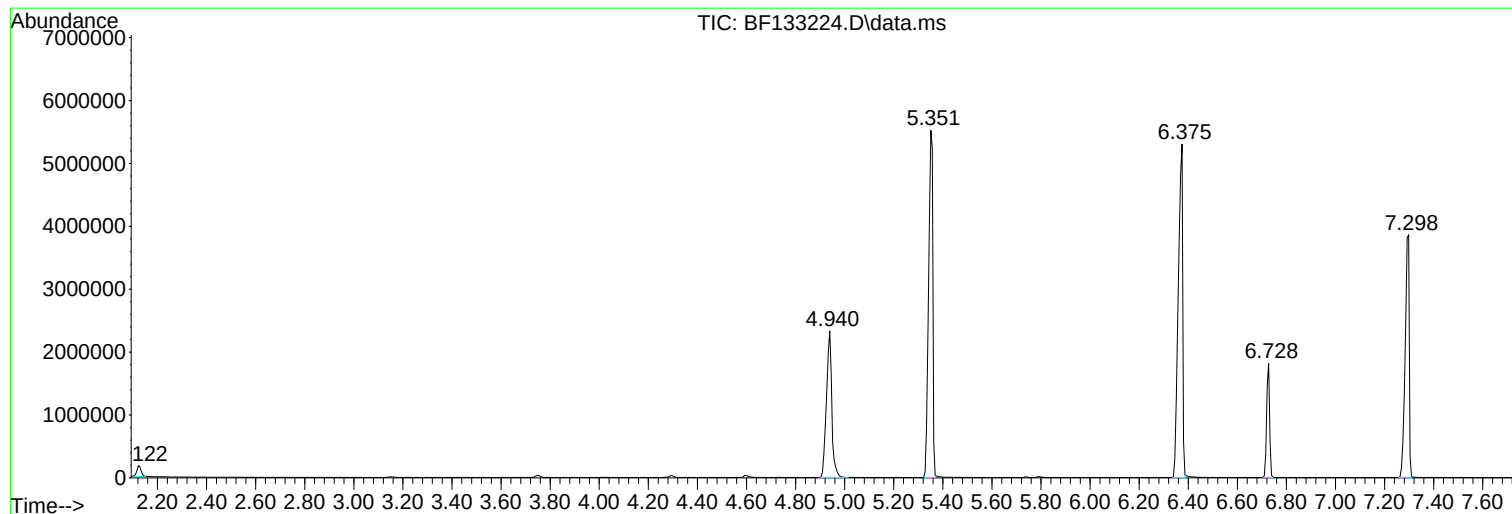
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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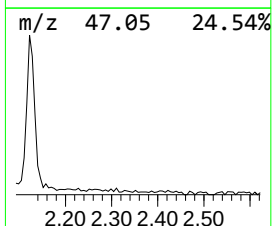
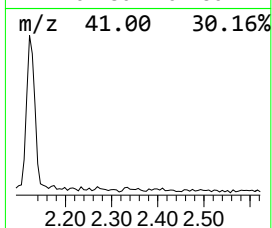
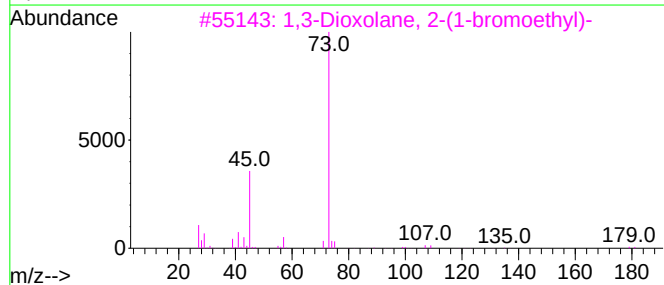
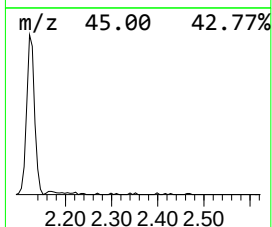
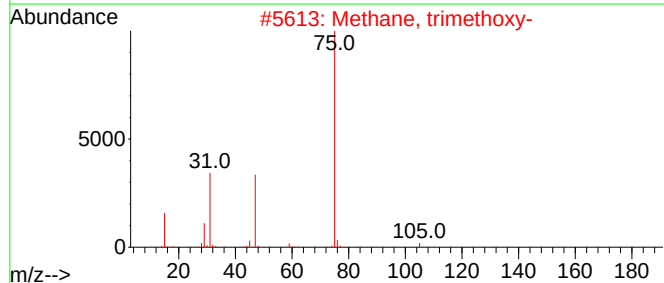
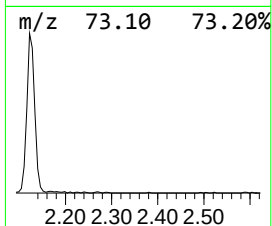
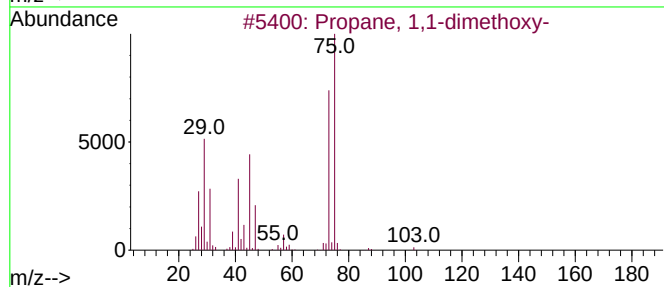
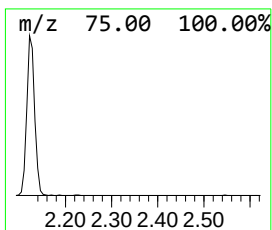
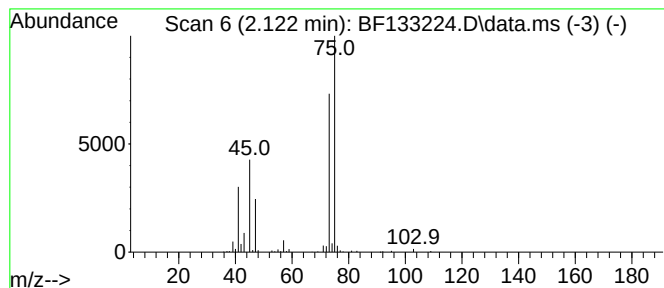
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	2.69 ng	202877	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
3			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
4			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	12
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10



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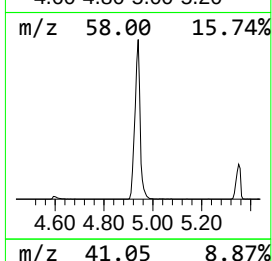
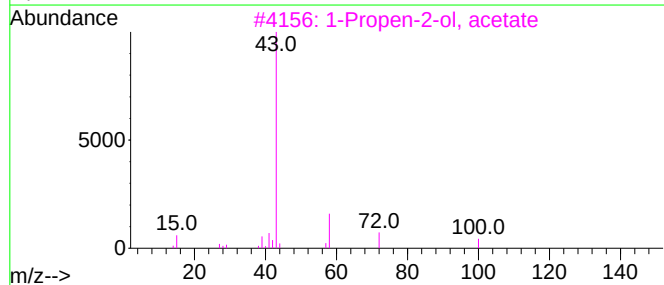
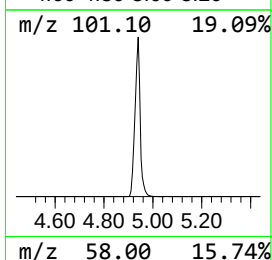
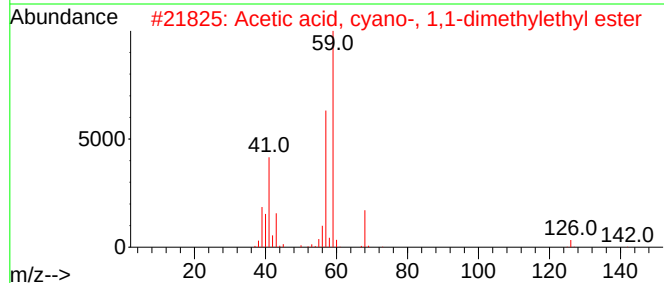
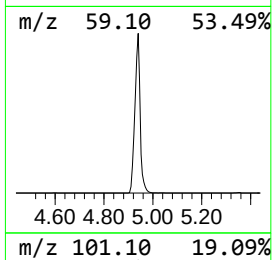
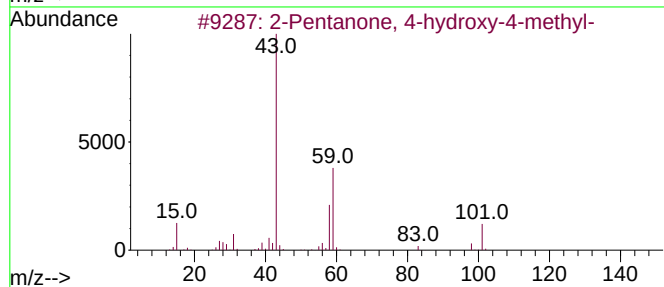
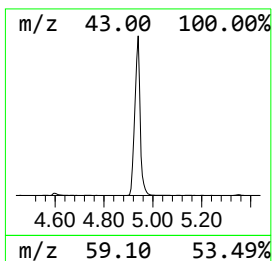
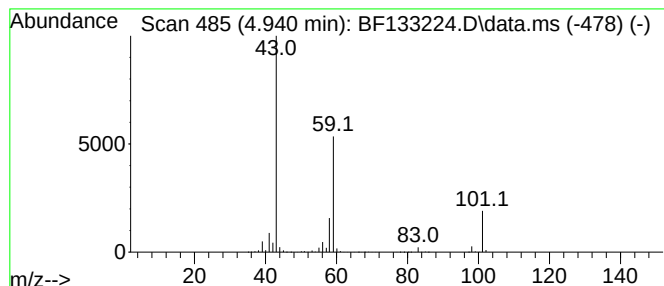
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.940	46.66 ng	3521590	1,4-Dichlorobenzene-d4			6.728
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
5	Propane, 1-ethoxy-2-methyl-		102	C6H14O	000627-02-1	9



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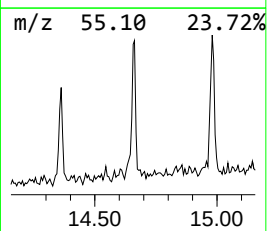
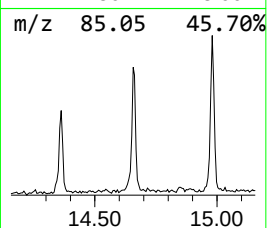
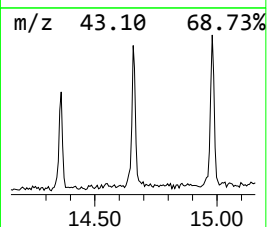
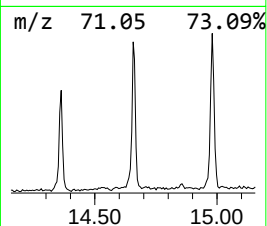
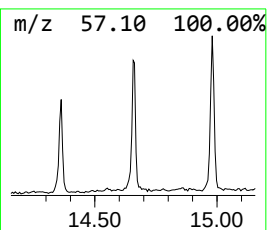
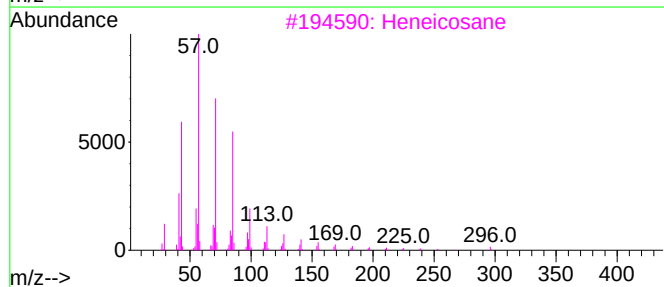
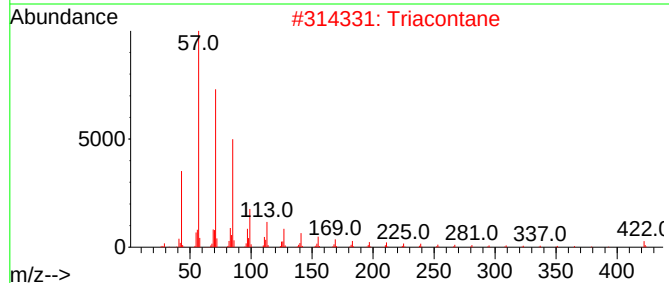
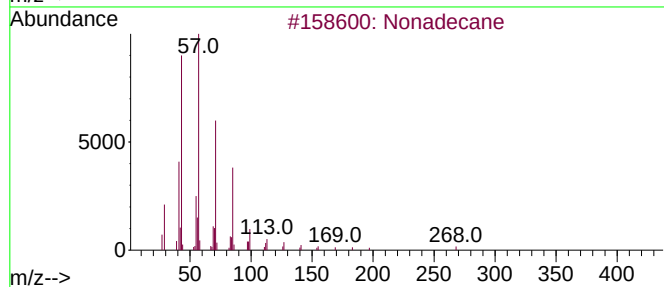
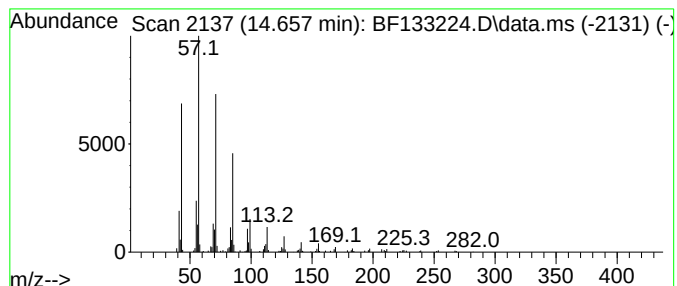
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	2.13 ng	179063	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	95
2			Triacontane	422	C30H62	000638-68-6	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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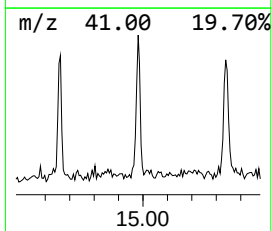
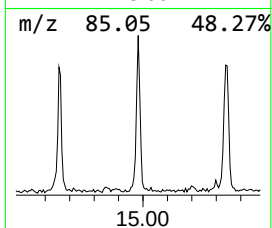
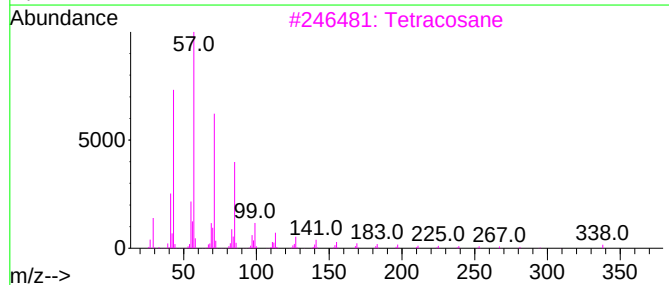
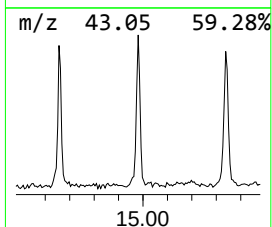
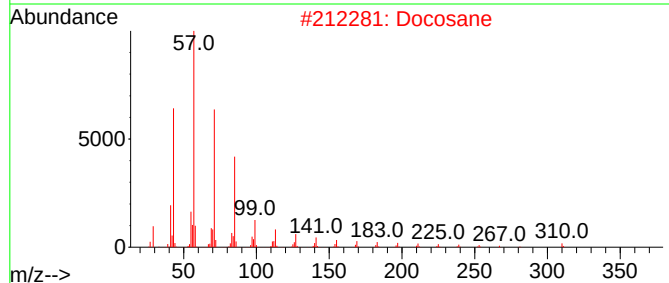
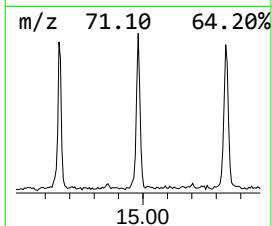
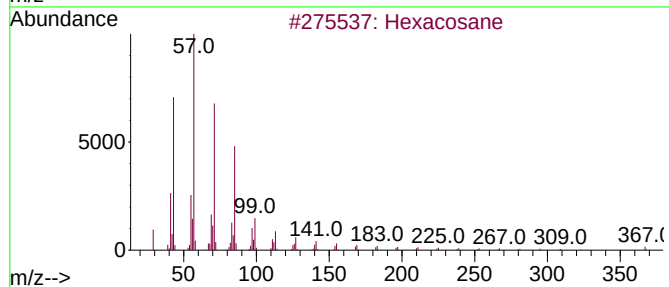
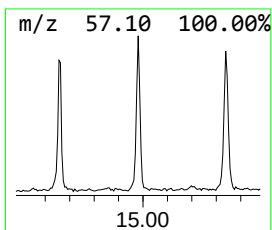
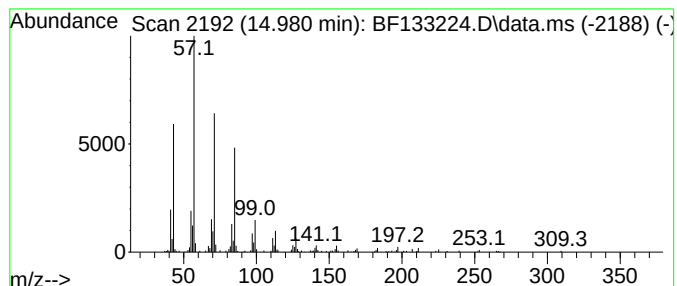
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	2.34 ng	197152	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Docosane	310	C22H46	000629-97-0	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	90



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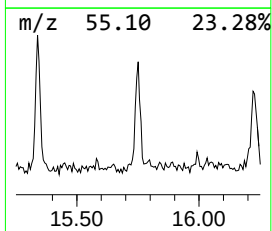
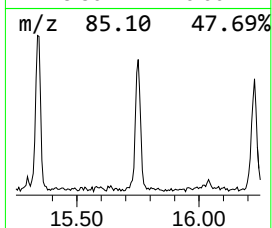
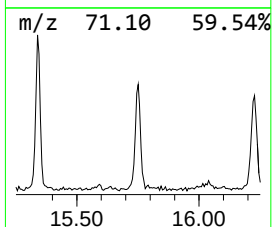
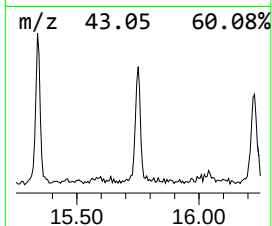
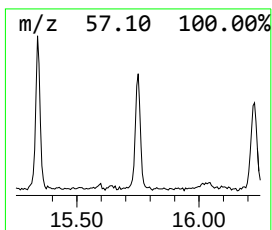
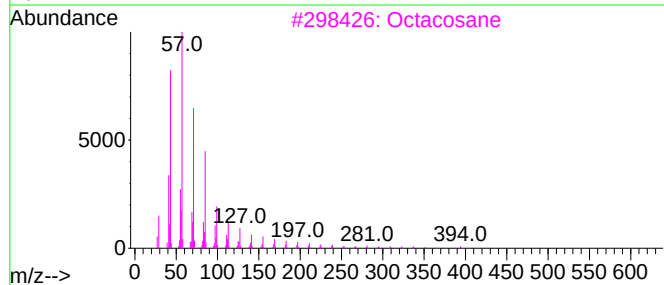
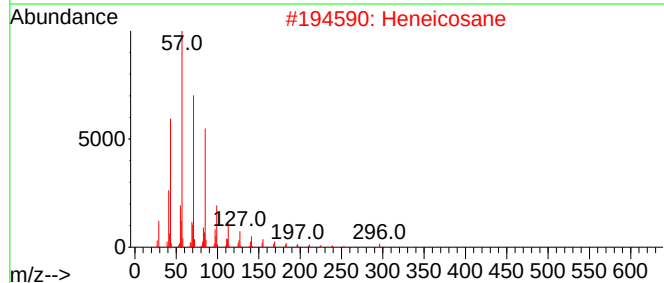
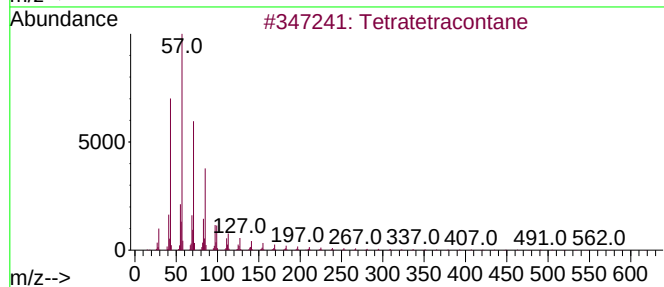
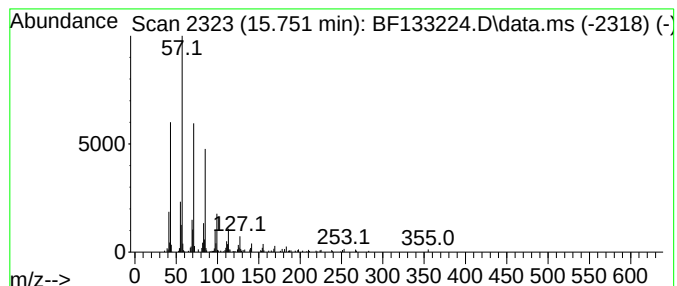
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	2.13 ng	179303	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			4-Methylheneicosane	310	C22H46	025117-29-7	91



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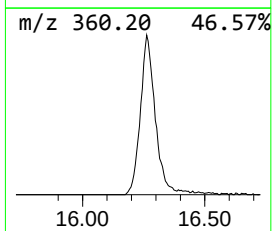
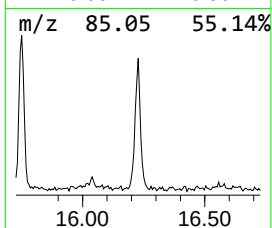
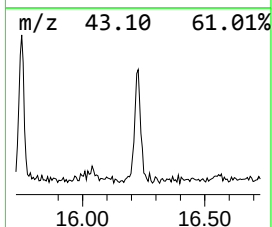
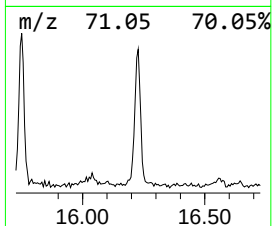
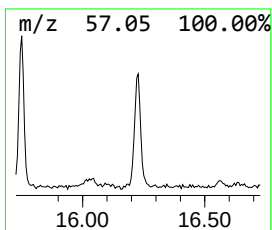
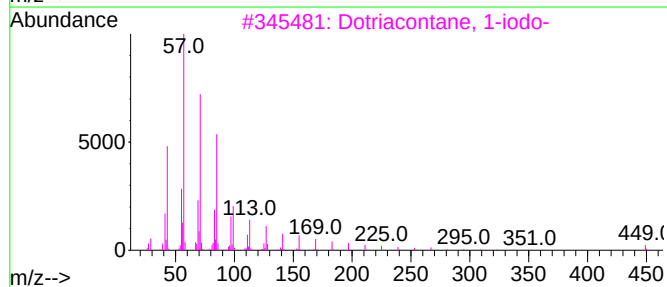
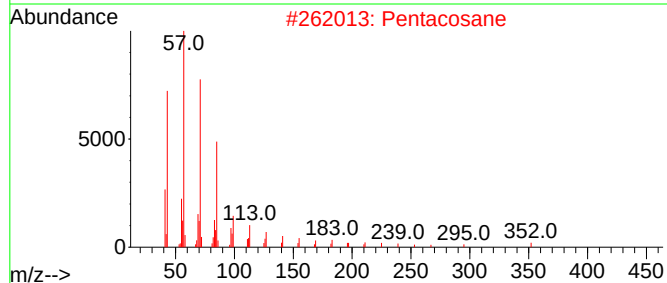
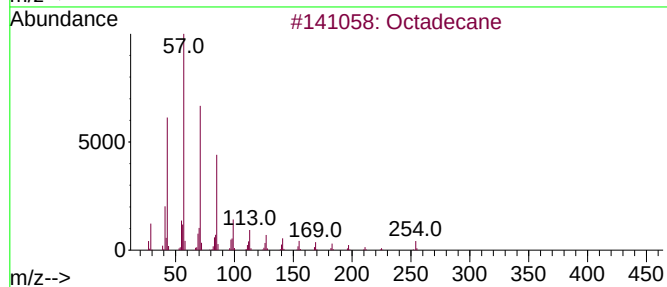
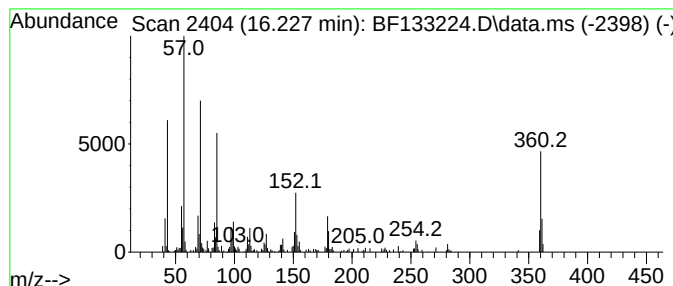
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.227	3.73 ng	313878	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	83
2			Pentacosane	352	C25H52	000629-99-2	42
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	42
4			Heneicosane	296	C21H44	000629-94-7	42
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133224.D
Acq On : 04 May 2023 11:07
Operator : CG\JU
Sample : PB152560BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152560BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Propane, 1,1-di...	2.122	2.7	ng	202877	1	6.728	1509470	20.0
2-Pentanone, 4-...	4.940	46.7	ng	3521590	1	6.728	1509470	20.0
Nonadecane	14.657	2.1	ng	179063	6	15.298	1683070	20.0
Hexacosane	14.980	2.3	ng	197152	6	15.298	1683070	20.0
Tetratetracontane	15.751	2.1	ng	179303	6	15.298	1683070	20.0
Octadecane	16.227	3.7	ng	313878	6	15.298	1683070	20.0