

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031924\
 Data File : BF137645.D
 Acq On : 19 Mar 2024 13:40
 Operator : CG\JU
 Sample : PB159655BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159655BL

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.946	482	486	501	rBV	161580	261279	4.19%	0.637%
2	5.351	550	555	577	rBV	4807177	5673147	91.00%	13.821%
3	6.369	723	728	731	rBV	4792680	5469094	87.73%	13.324%
4	6.722	785	788	806	rBV	1250870	1256502	20.16%	3.061%
5	7.292	880	885	888	rBV	3503735	3527553	56.59%	8.594%
6	8.004	1002	1006	1024	rBV	1711361	1695540	27.20%	4.131%
7	9.086	1184	1190	1193	rBV	6402269	6234000	100.00%	15.187%
8	9.757	1300	1304	1318	rBV	2149841	1906069	30.58%	4.643%
9	10.551	1434	1439	1463	rBV	3463047	3678917	59.01%	8.962%
10	11.239	1553	1556	1567	rBV	2063409	1828415	29.33%	4.454%
11	12.651	1792	1796	1800	rBV	189016	159313	2.56%	0.388%
12	12.833	1822	1827	1830	rBV	5872829	6103220	97.90%	14.868%
13	13.357	1912	1916	1921	rBV	143811	128493	2.06%	0.313%
14	13.874	2000	2004	2017	rBV	1336774	1331701	21.36%	3.244%
15	14.651	2131	2136	2140	rBV	78405	84014	1.35%	0.205%
16	14.968	2186	2190	2196	rBV	104844	112720	1.81%	0.275%
17	15.298	2241	2246	2250	rBV	813993	1066884	17.11%	2.599%
18	15.745	2317	2322	2329	rBV	103793	148609	2.38%	0.362%
19	16.215	2396	2402	2409	rBV	89066	155146	2.49%	0.378%
20	16.774	2490	2497	2504	rBV2	56378	120798	1.94%	0.294%
21	17.427	2601	2608	2618	rBV2	40796	106964	1.72%	0.261%

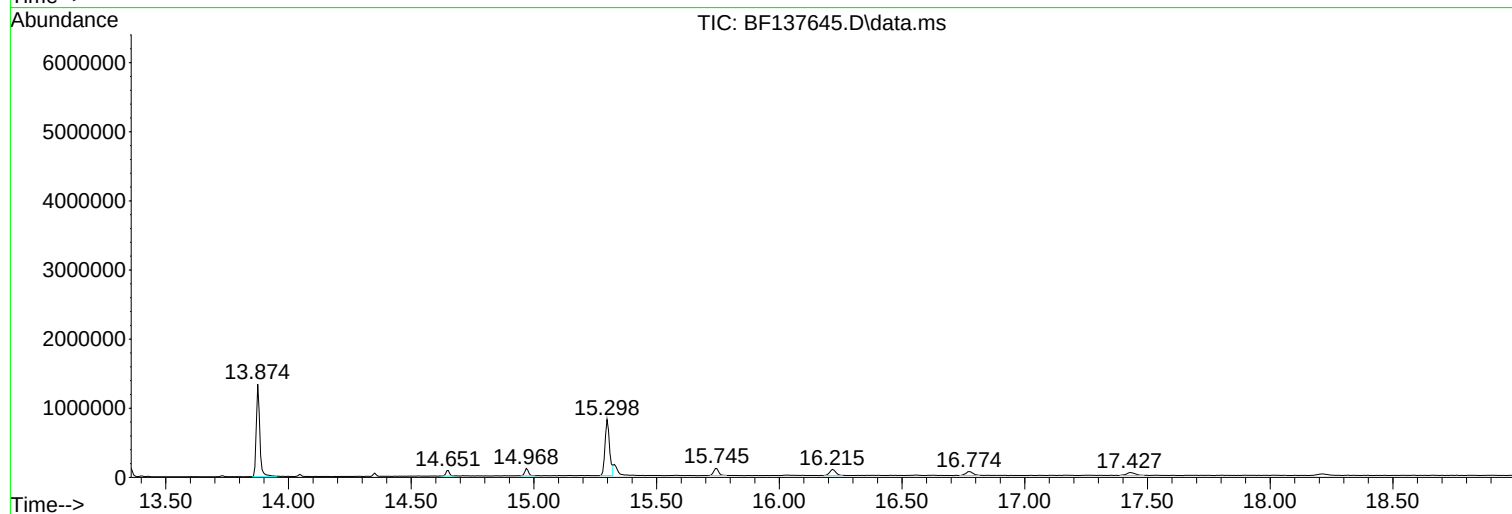
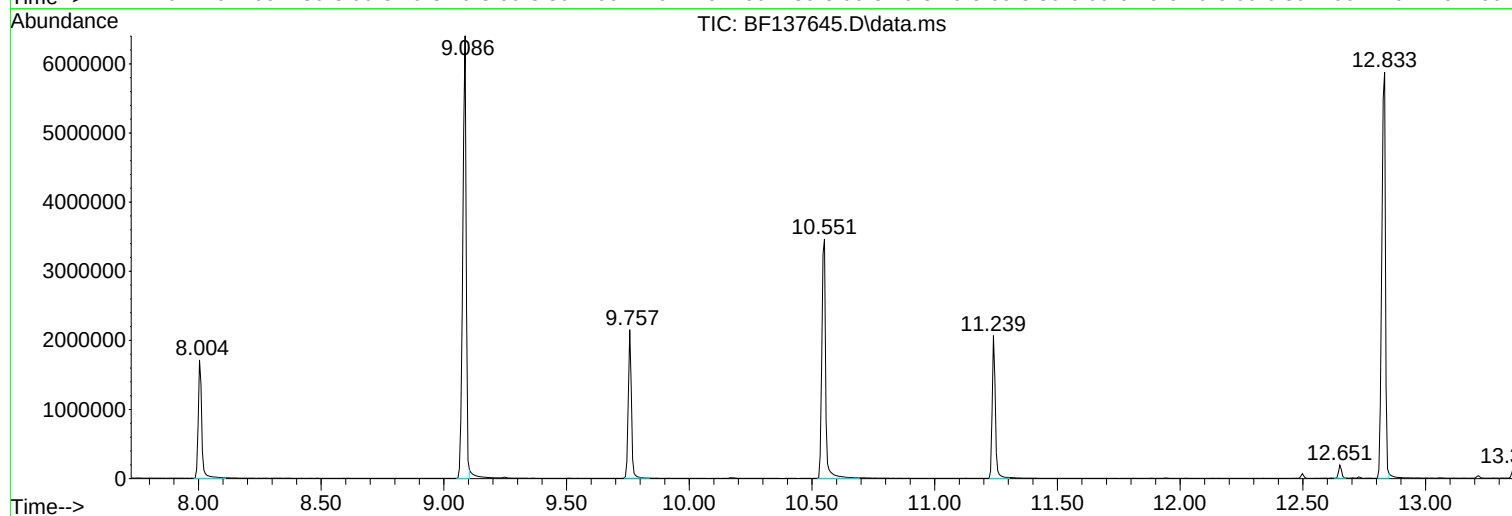
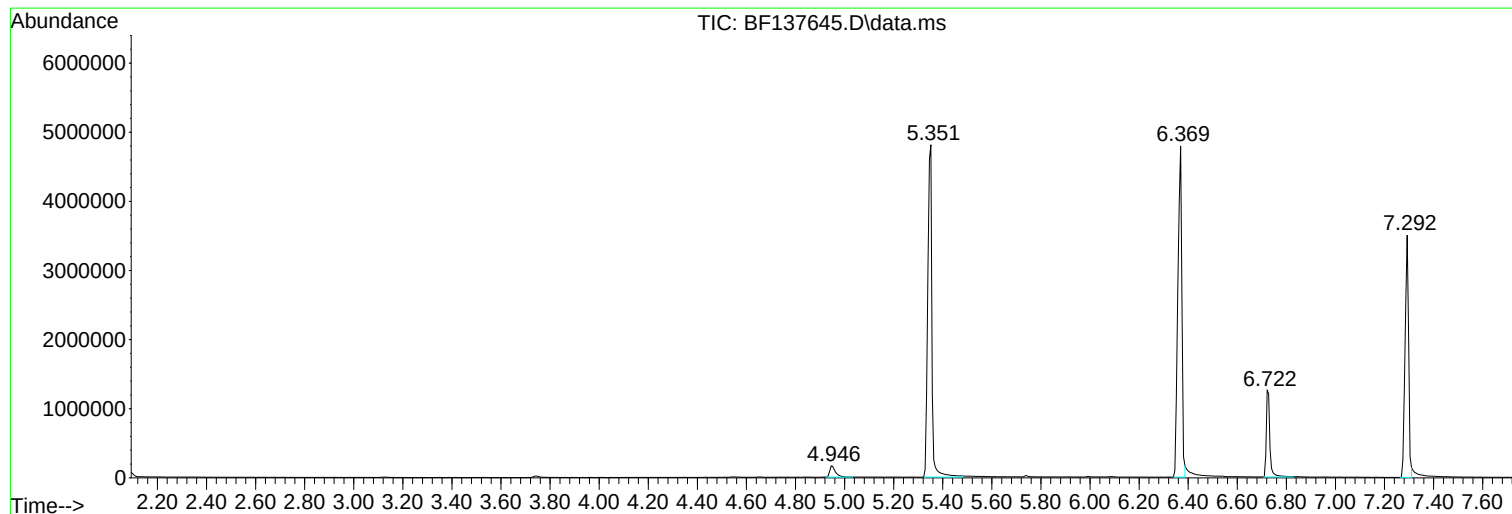
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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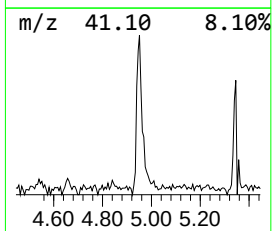
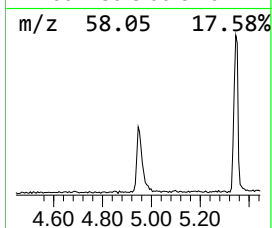
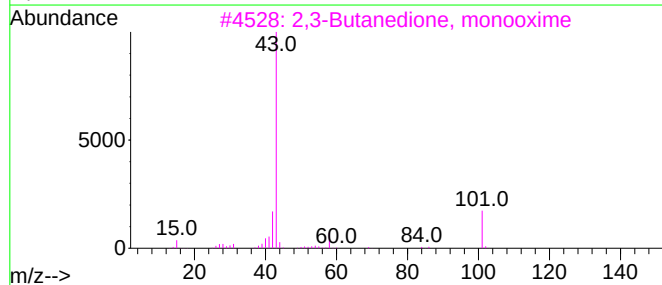
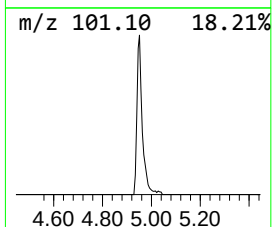
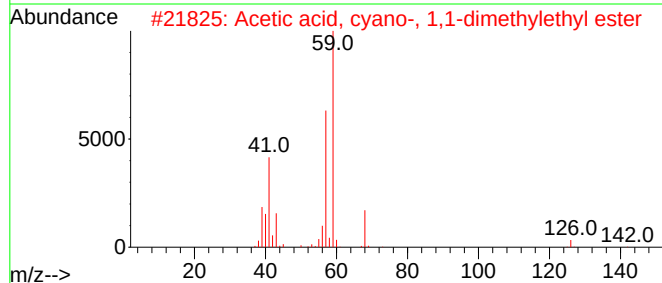
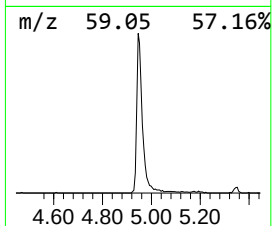
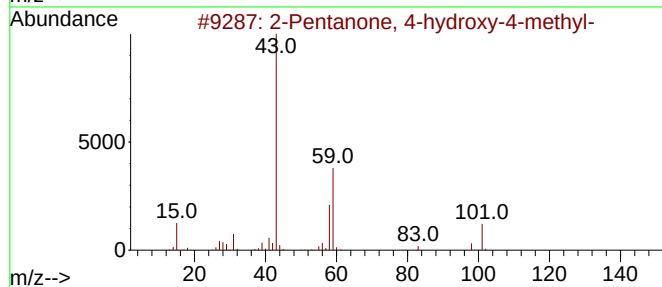
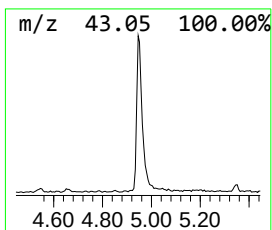
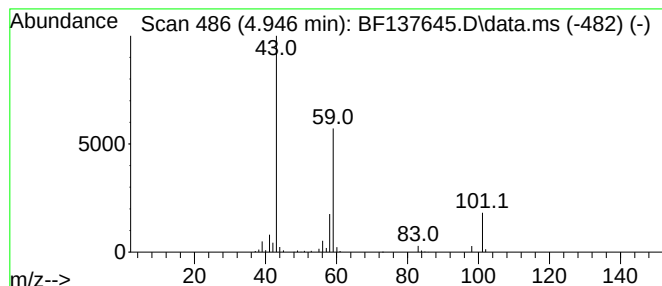
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	4.16 ng	261279	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	59	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	10	



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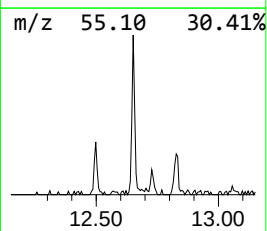
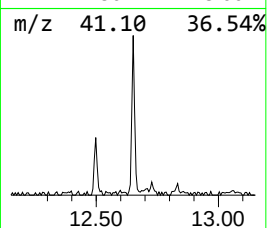
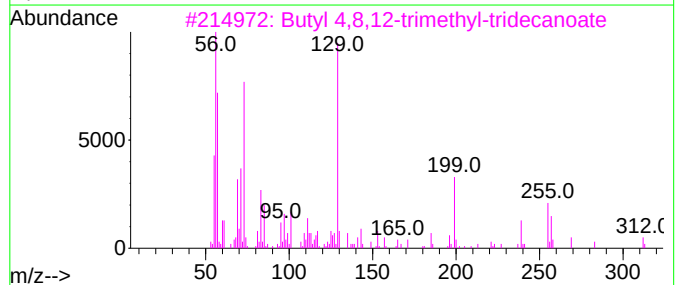
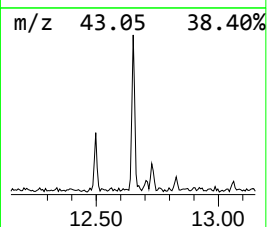
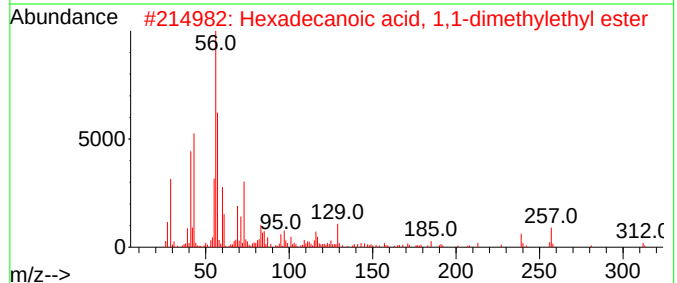
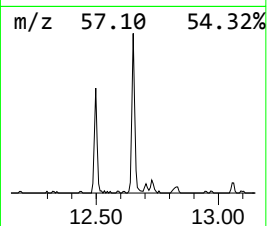
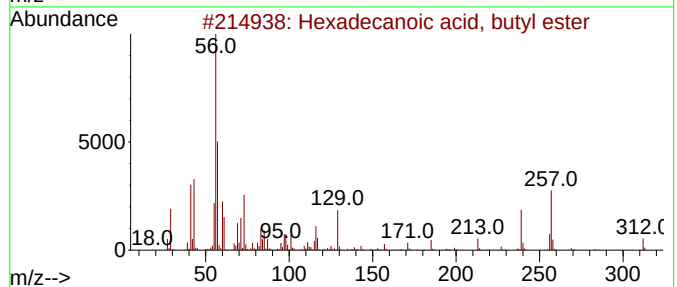
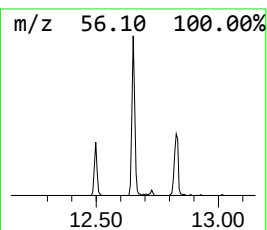
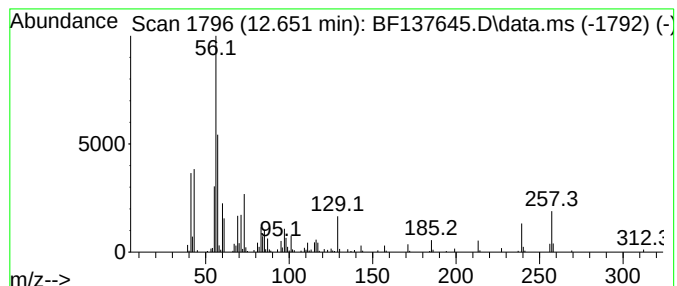
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.39 ng	159313	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	60
3			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	50
4			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38
5			Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37



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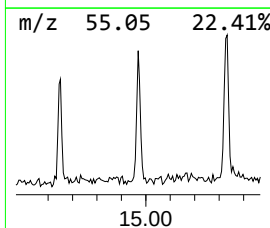
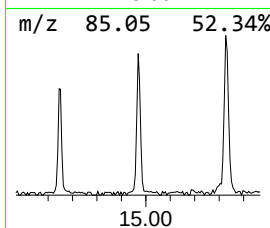
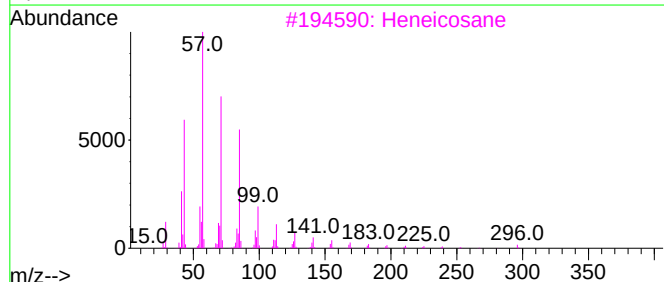
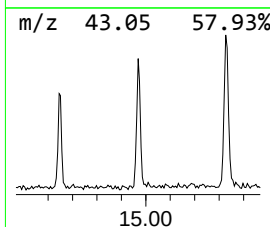
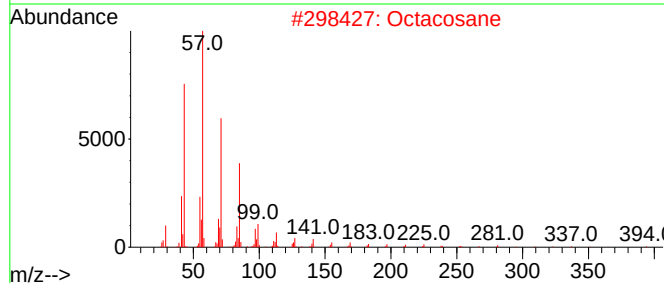
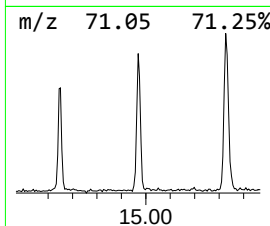
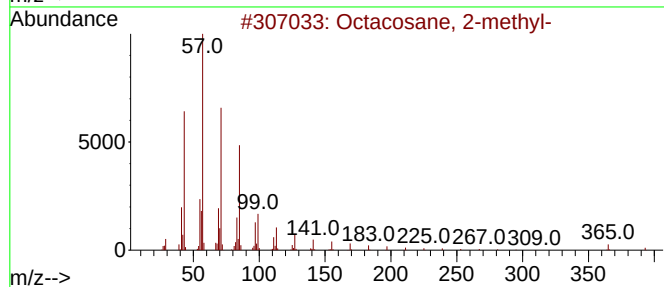
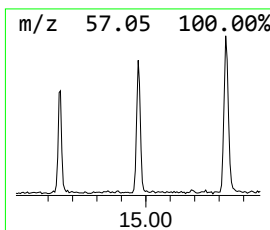
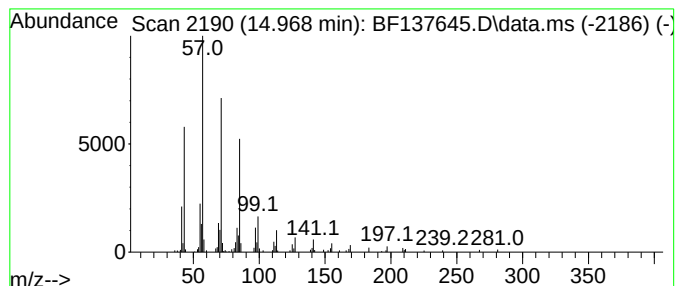
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Peak Number 3 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.969	2.11 ng	112720	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Tetratetracontane	619	C44H90	007098-22-8	91



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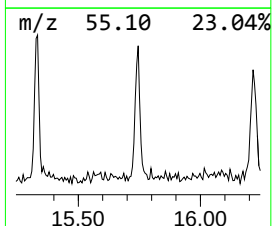
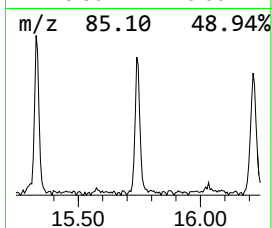
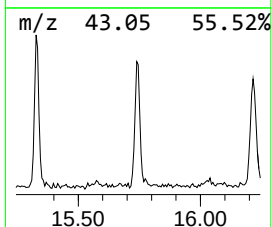
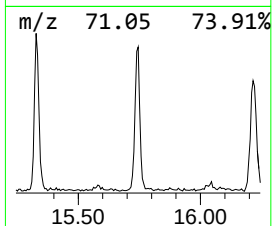
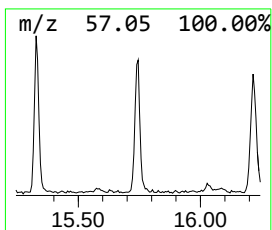
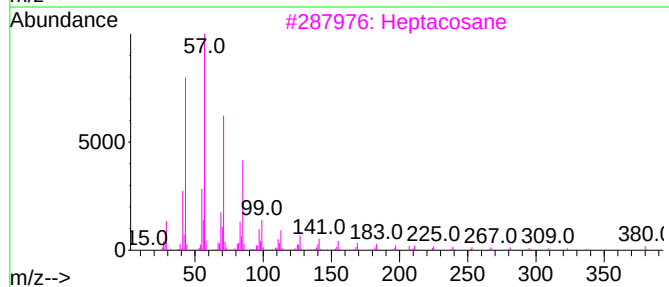
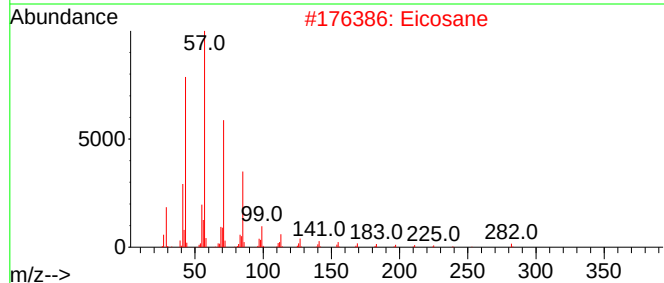
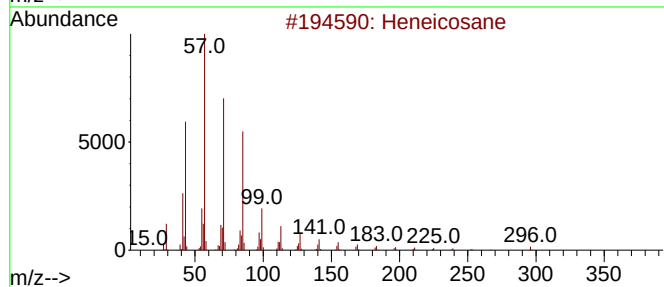
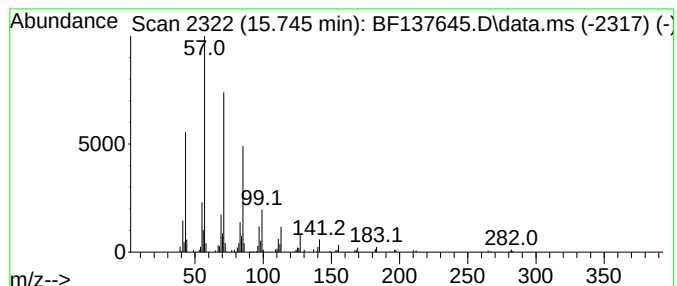
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Peak Number 4 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	2.79 ng	148609	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Eicosane	282	C20H42	000112-95-8	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90



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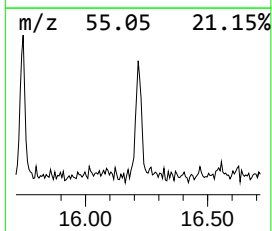
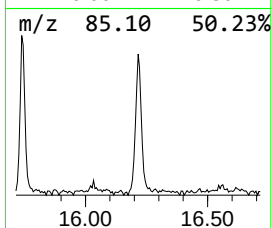
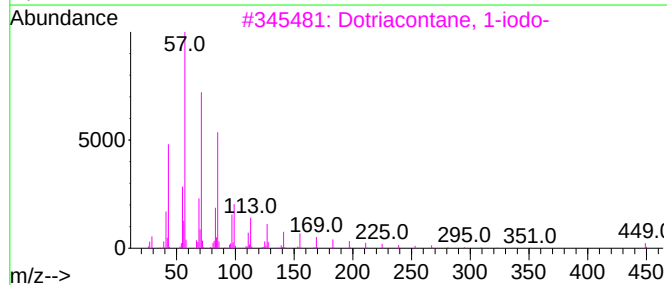
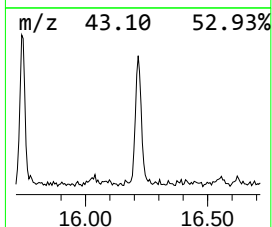
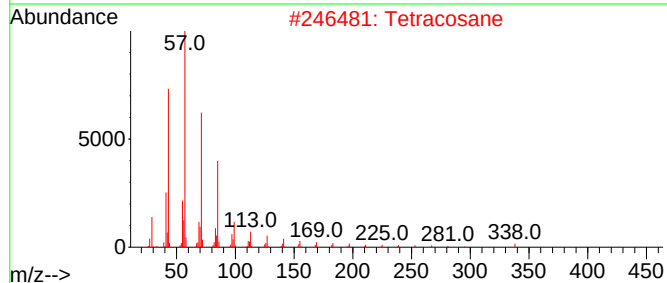
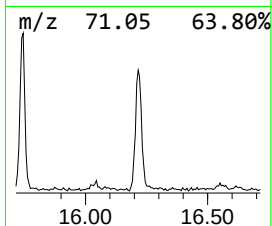
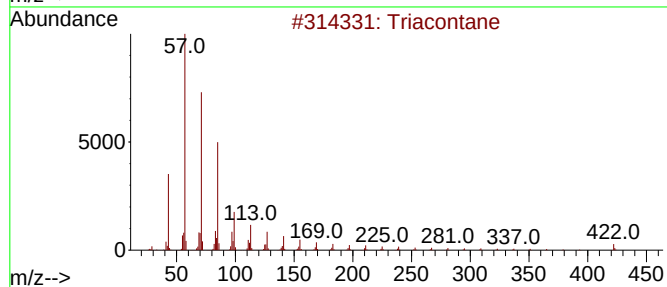
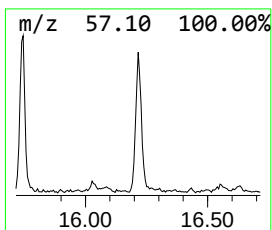
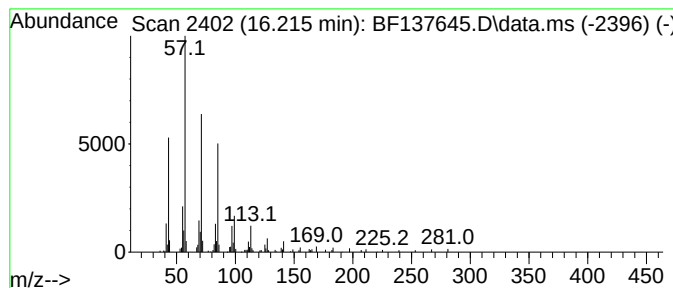
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Peak Number 5 Triacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	2.91 ng	155146	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Octacosane	394	C28H58	000630-02-4	91



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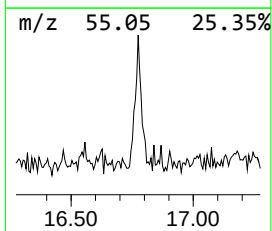
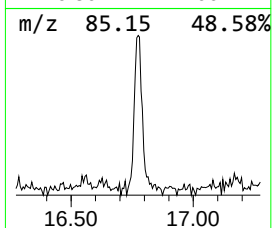
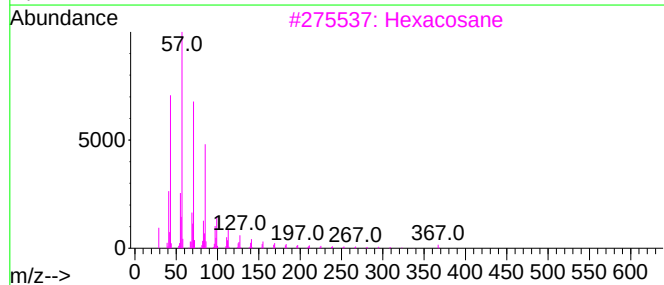
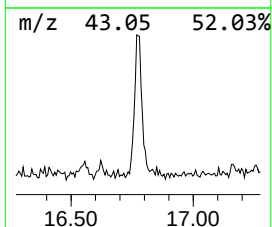
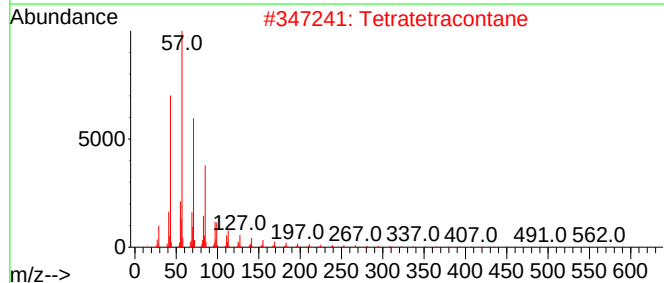
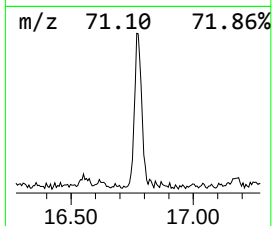
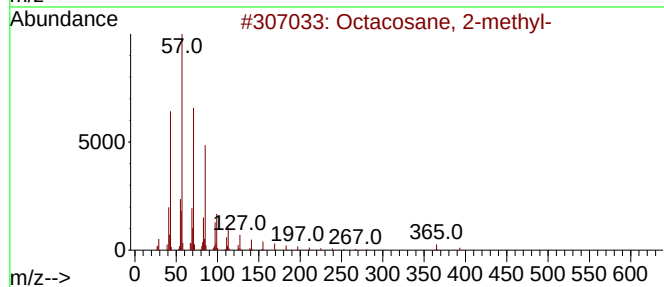
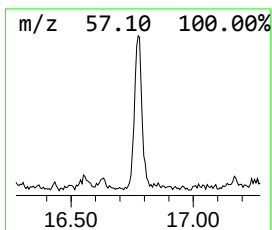
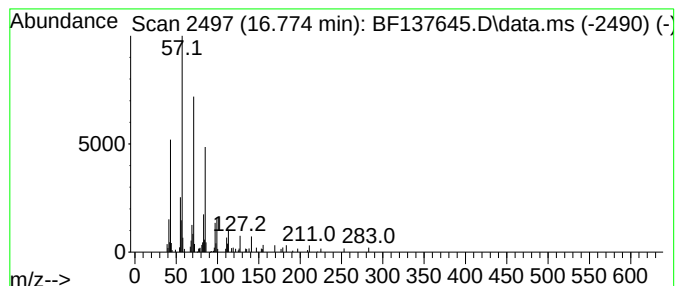
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	2.26 ng	120798	Perylene-d12	15.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031924\
Data File : BF137645.D
Acq On : 19 Mar 2024 13:40
Operator : CG\JU
Sample : PB159655BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159655BL

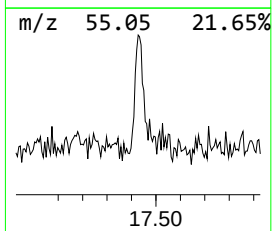
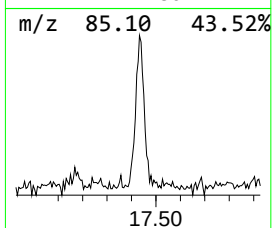
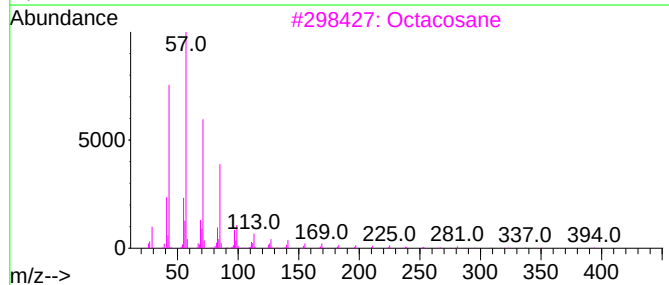
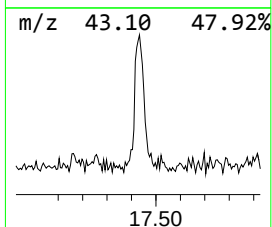
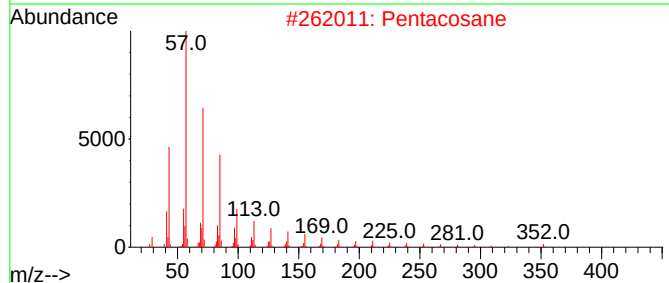
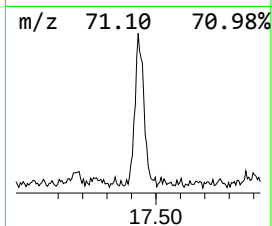
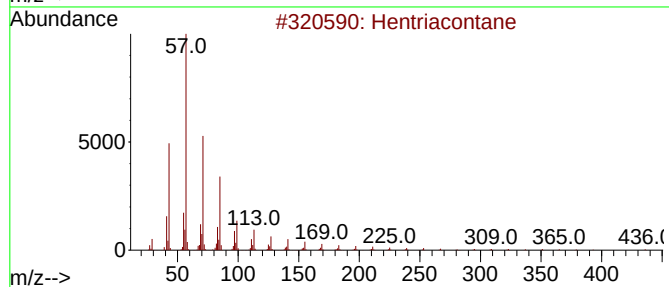
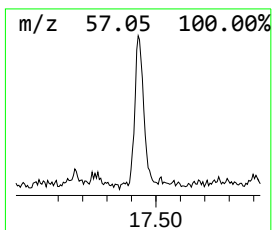
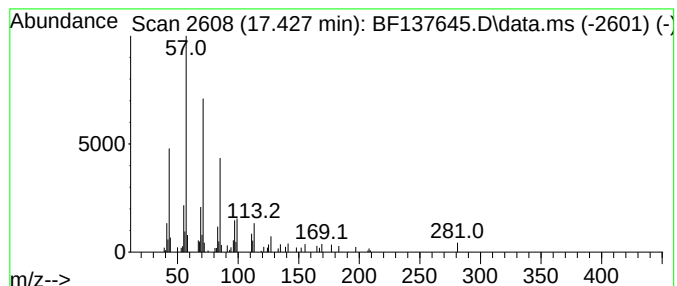
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.427	2.01 ng	106964	Perylene-d12	15.298

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	87
2		Pentacosane	352	C25H52	000629-99-2	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Heneicosane	296	C21H44	000629-94-7	83
5		Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031924\
Data File : BF137645.D
Acq On : 19 Mar 2024 13:40
Operator : CG\JU
Sample : PB159655BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159655BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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-...	4.946	4.2	ng	261279	1	6.728	1256500	20.0
Hexadecanoic ac...	12.651	2.4	ng	159313	5	13.874	1331700	20.0
Octacosane, 2-m...	14.969	2.1	ng	112720	6	15.298	1066880	20.0
Heneicosane	15.745	2.8	ng	148609	6	15.298	1066880	20.0
Triacontane	16.215	2.9	ng	155146	6	15.298	1066880	20.0
Tetratetracontane	16.774	2.3	ng	120798	6	15.298	1066880	20.0
Hentriacontane	17.427	2.0	ng	106964	6	15.298	1066880	20.0