

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051623\
 Data File : BF133398.D
 Acq On : 16 May 2023 12:49
 Operator : CG\JU
 Sample : PB152835BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB152835BL

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: BF133398.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	477	483	499	rBV	2629450	4139881	48.18%	6.469%
2	5.351	549	555	558	rBV	6896014	7548260	87.85%	11.794%
3	6.375	723	729	732	rBV	6461051	7597268	88.42%	11.871%
4	6.722	784	788	791	rBV	2071240	1814524	21.12%	2.835%
5	7.293	879	885	888	rBV	4991833	5104706	59.41%	7.976%
6	8.004	1001	1006	1010	rBV	3041472	2554034	29.72%	3.991%
7	9.087	1183	1190	1193	rBV	8325548	8326892	96.91%	13.011%
8	9.757	1298	1304	1307	rBV	3711211	2981690	34.70%	4.659%
9	10.551	1434	1439	1442	rBV	4711159	5068213	58.98%	7.919%
10	11.245	1552	1557	1560	rBV	3234266	3025082	35.21%	4.727%
11	12.833	1822	1827	1830	rBV	7339955	8592520	100.00%	13.426%
12	13.363	1913	1917	1921	rBV	147972	141087	1.64%	0.220%
13	13.880	2001	2005	2014	rBV	2507421	2285768	26.60%	3.572%
14	14.357	2082	2086	2091	rBV	155314	141641	1.65%	0.221%
15	14.651	2133	2136	2140	rVB	280581	269278	3.13%	0.421%
16	14.974	2187	2191	2197	rBV	357193	370065	4.31%	0.578%
17	15.304	2242	2247	2250	rBV	1518337	1781231	20.73%	2.783%
18	15.333	2250	2252	2260	rVB	399341	434152	5.05%	0.678%
19	15.745	2317	2322	2328	rBV	294877	420017	4.89%	0.656%
20	16.215	2397	2402	2407	rBV	253613	491395	5.72%	0.768%
21	16.774	2491	2497	2504	rVB3	171916	348033	4.05%	0.544%
22	17.427	2601	2608	2615	rBV2	145143	337549	3.93%	0.527%
23	18.204	2735	2740	2751	rVB3	83903	225174	2.62%	0.352%

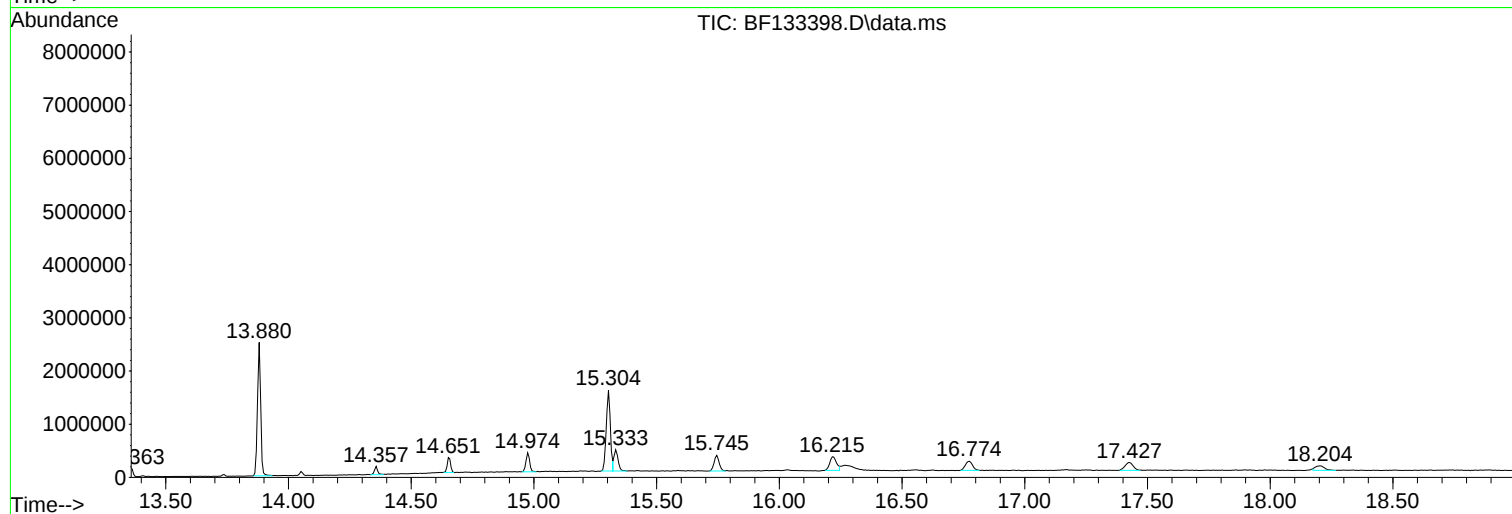
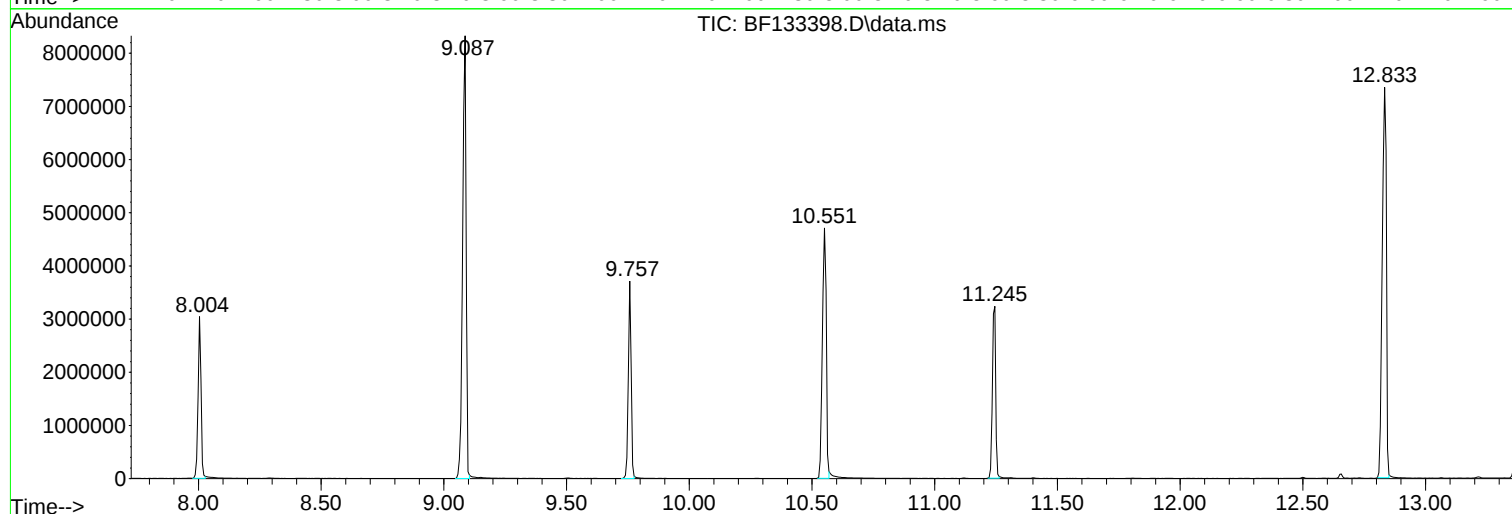
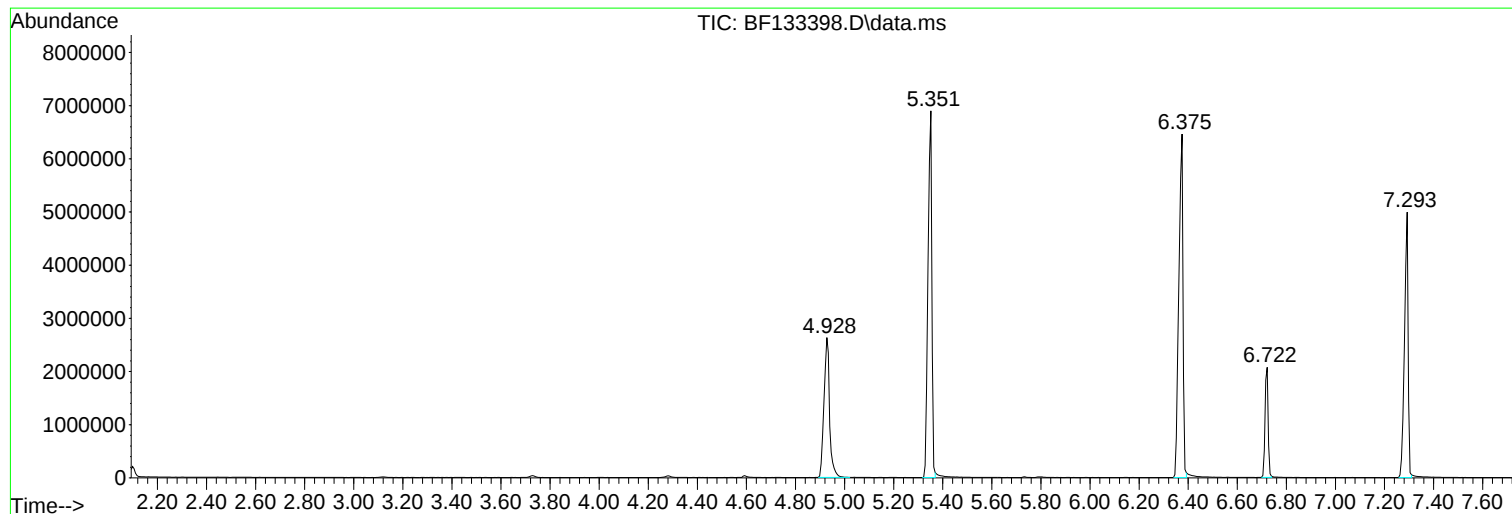
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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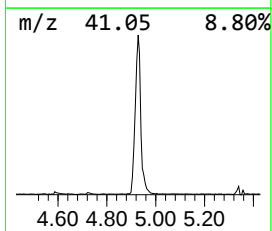
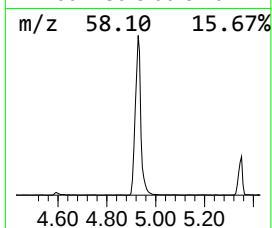
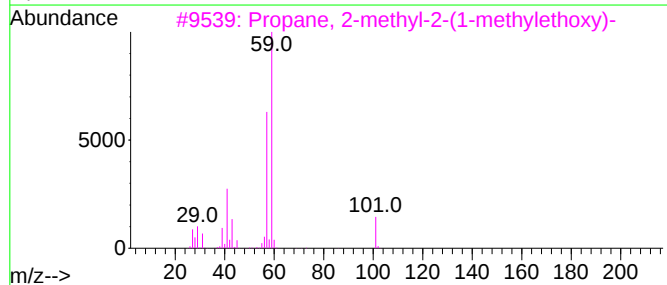
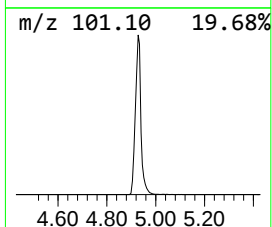
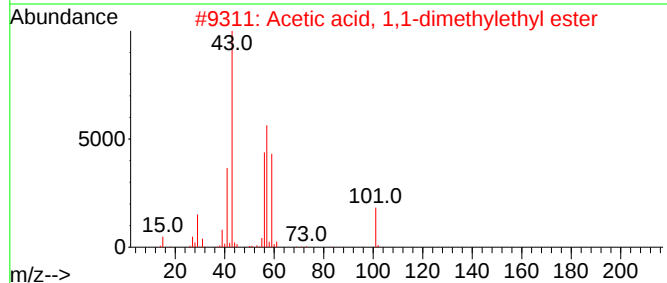
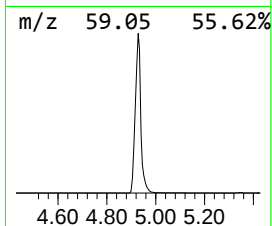
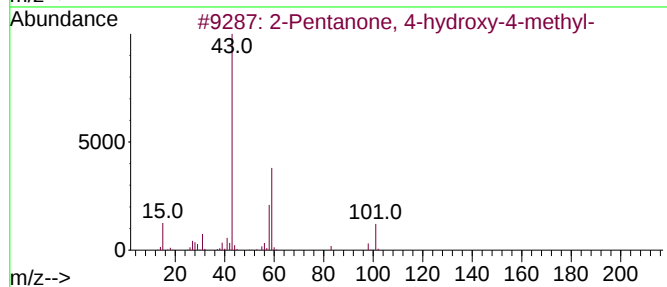
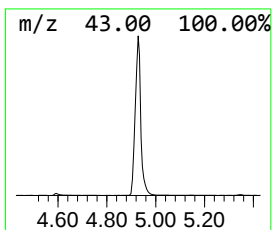
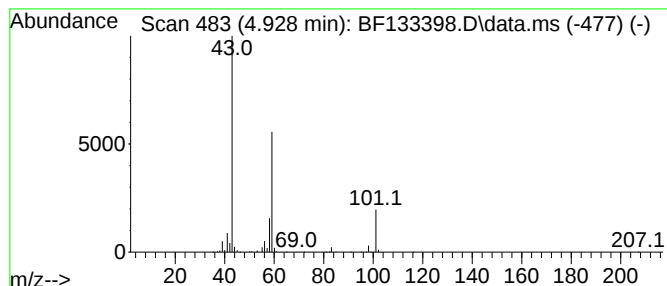
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.928	45.63 ng	4139880	1,4-Dichlorobenzene-d4	6.722	
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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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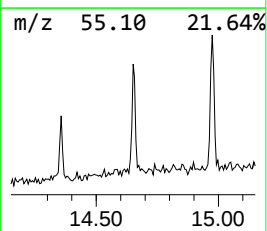
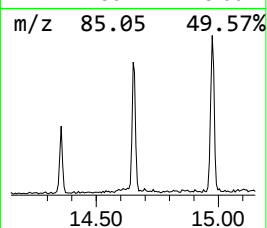
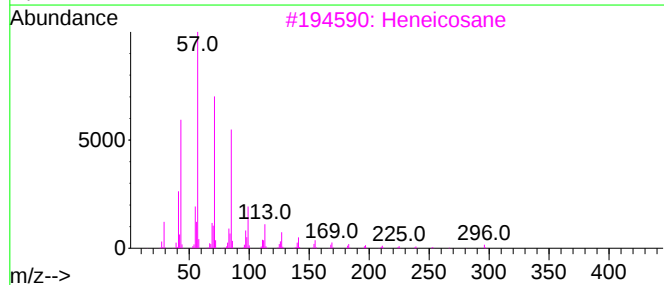
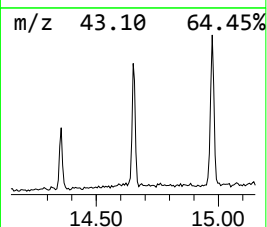
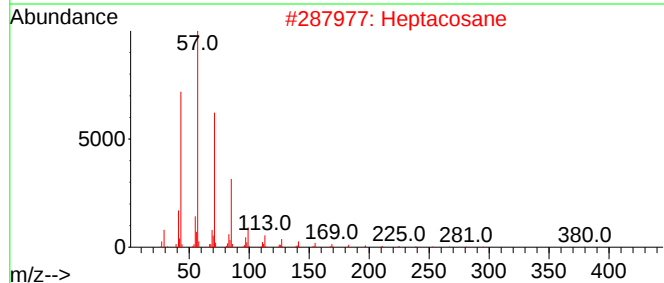
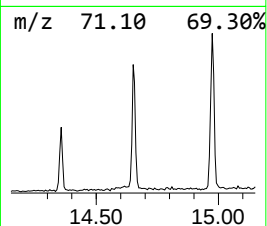
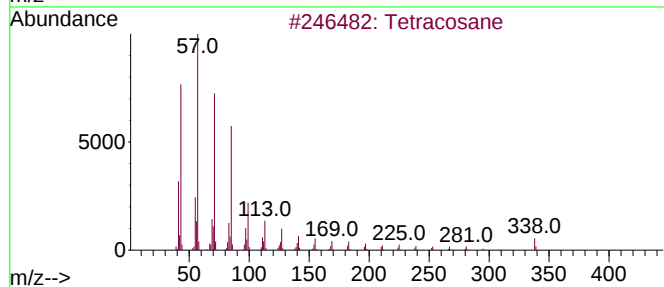
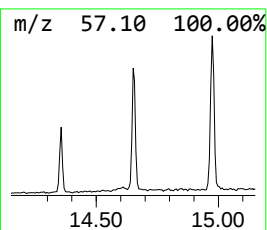
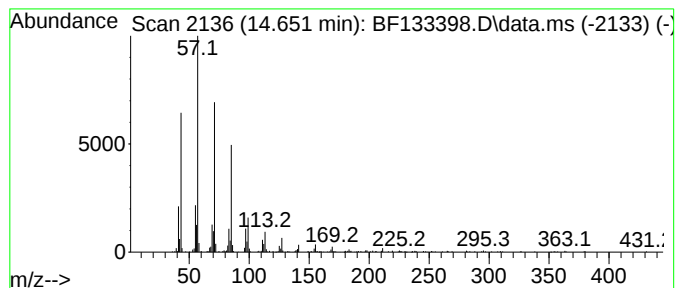
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	3.02 ng	269278	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	95
2		Heptacosane	380	C27H56	000593-49-7	95
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane	310	C22H46	000629-97-0	91
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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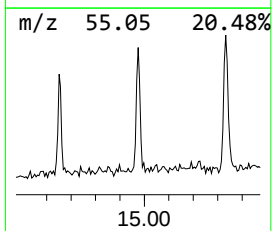
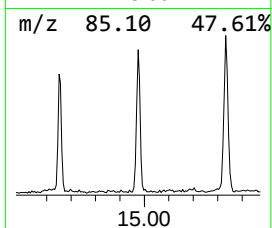
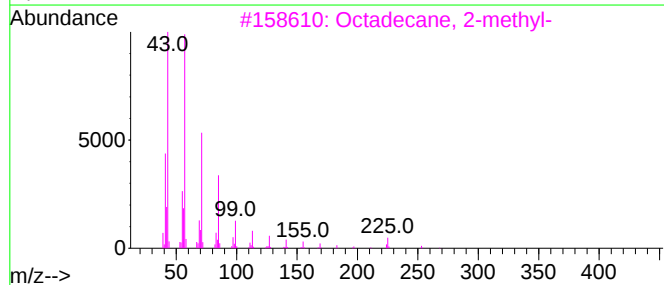
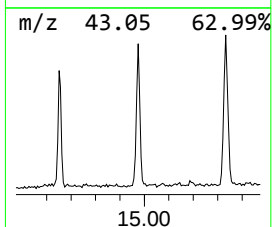
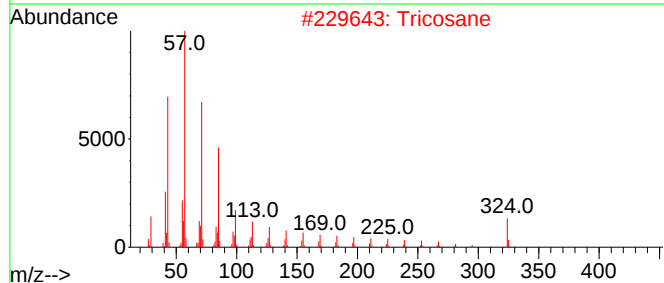
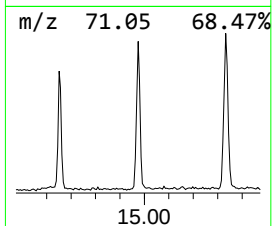
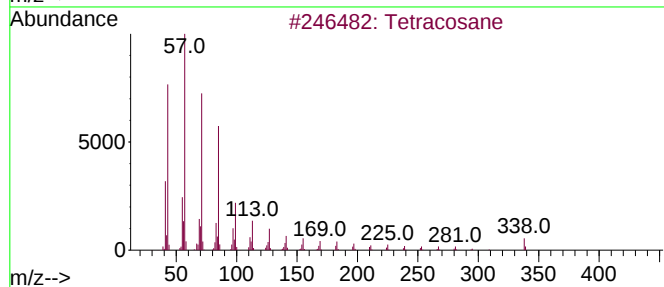
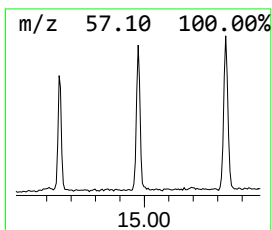
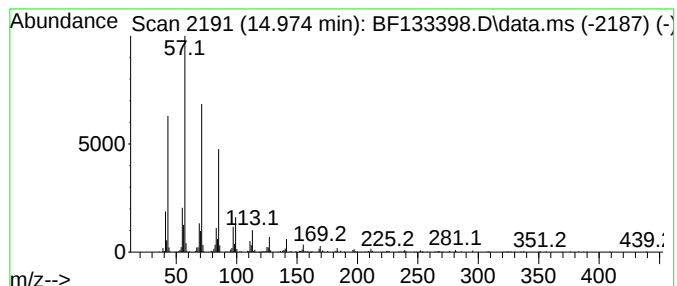
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tricosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	4.16 ng	370065	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	97
2			Tricosane	324	C23H48	000638-67-5	93
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
4			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
5			Octacosane	394	C28H58	000630-02-4	91



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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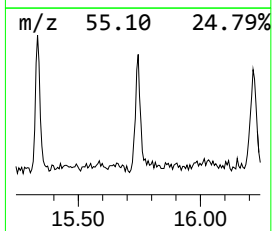
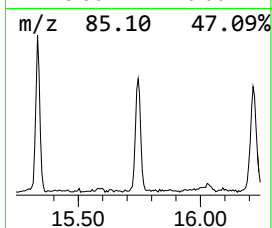
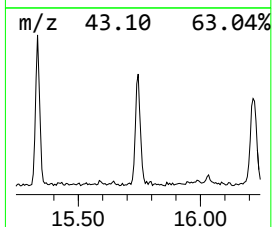
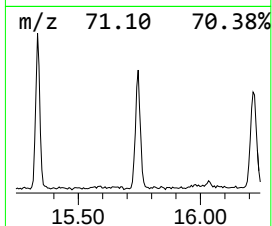
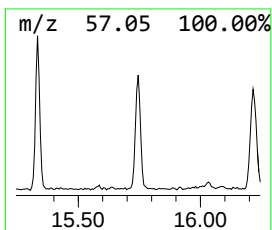
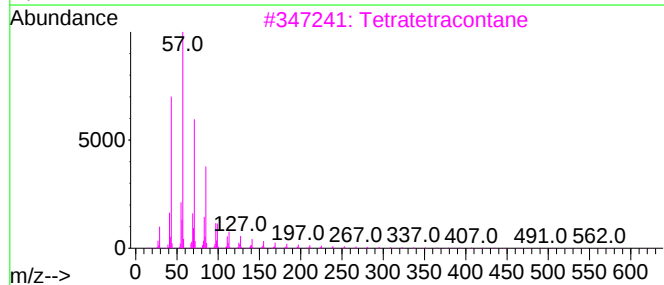
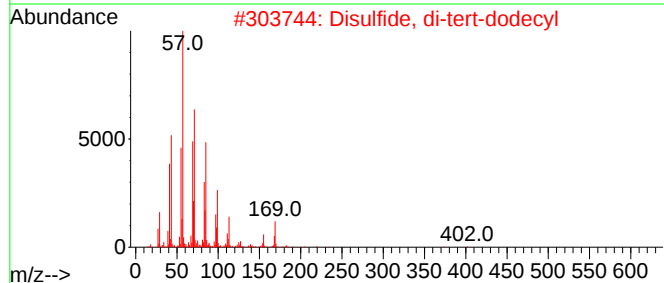
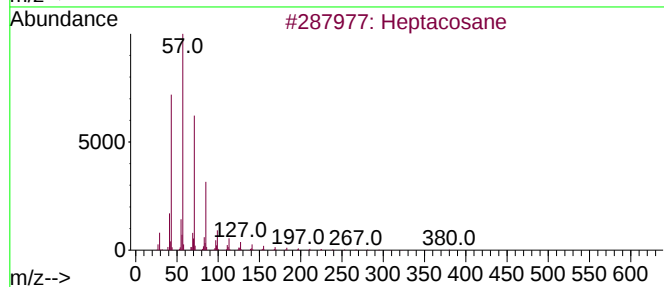
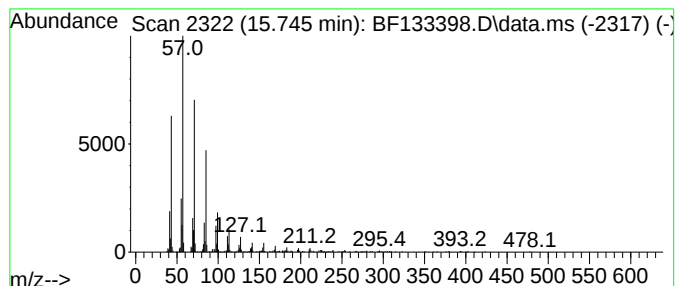
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Peak Number 4 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	4.72 ng	420017	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	95
2			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	94
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Hexacosane	366	C26H54	000630-01-3	90



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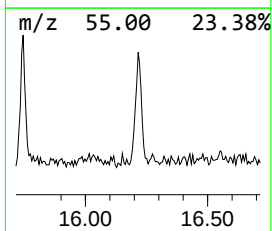
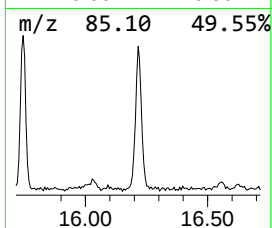
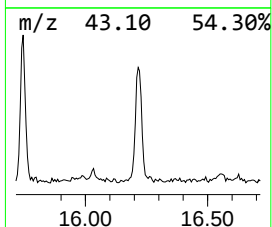
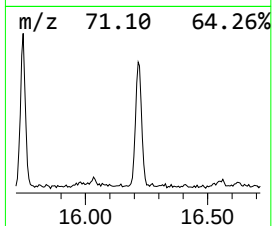
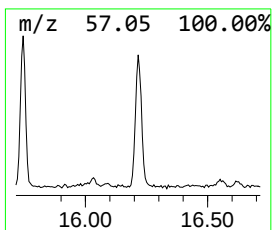
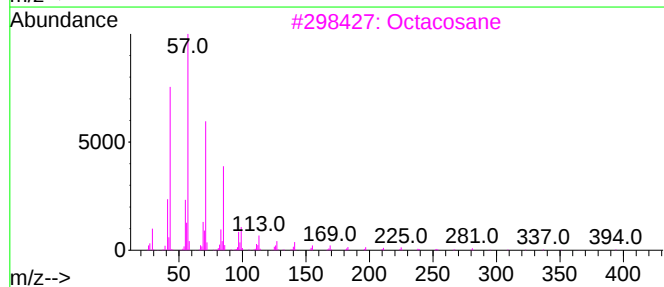
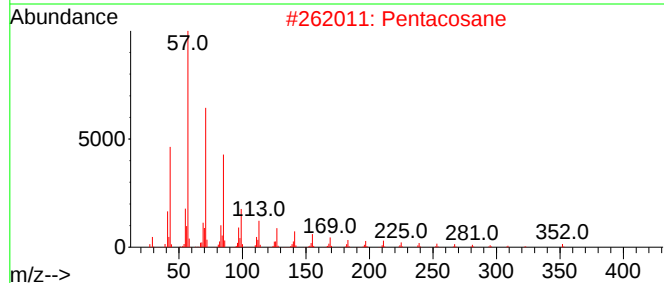
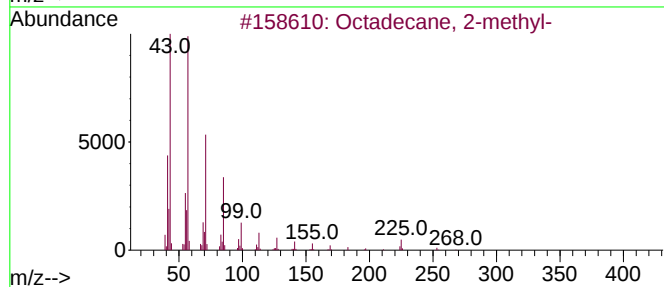
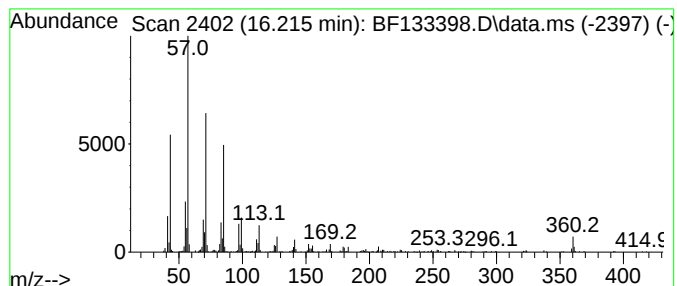
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	5.52 ng	491395	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
2			Pentacosane	352	C25H52	000629-99-2	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5			Hentriacontane	437	C31H64	000630-04-6	87



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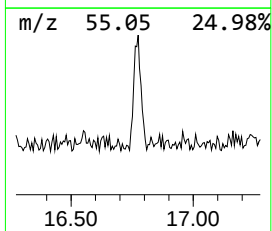
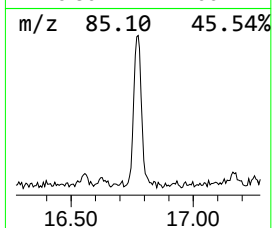
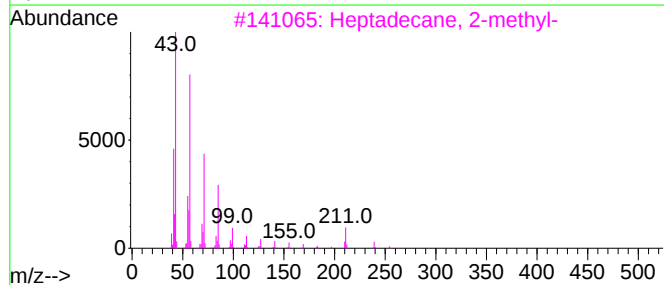
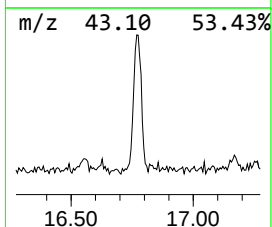
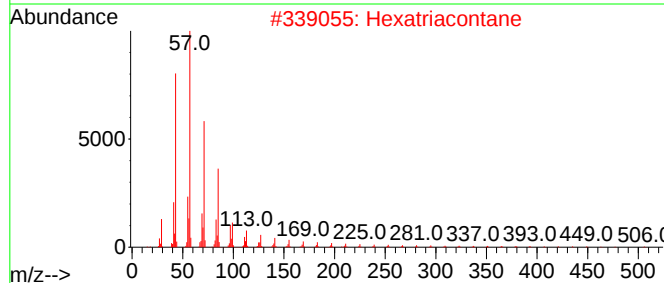
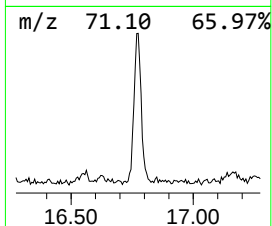
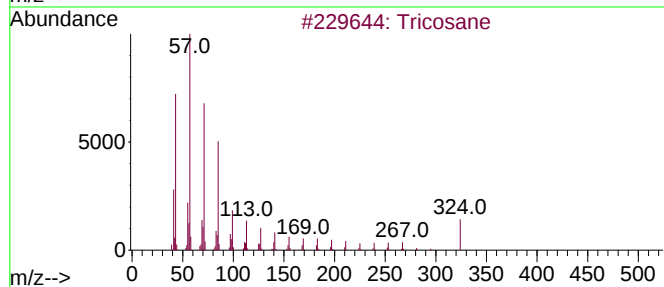
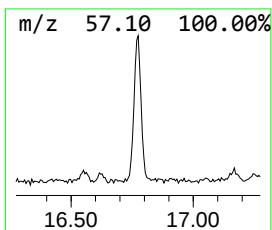
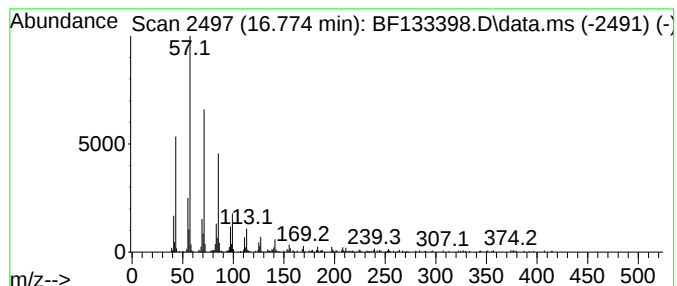
Instrument :
BNA_F
ClientSampleId :
PB152835BL

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 Hexatriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.774	3.91 ng	348033	Perylene-d12	15.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Hexatriacontane	507	C36H74	000630-06-8	91
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051623\
Data File : BF133398.D
Acq On : 16 May 2023 12:49
Operator : CG\JU
Sample : PB152835BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152835BL

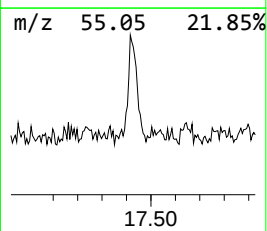
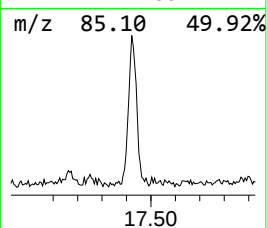
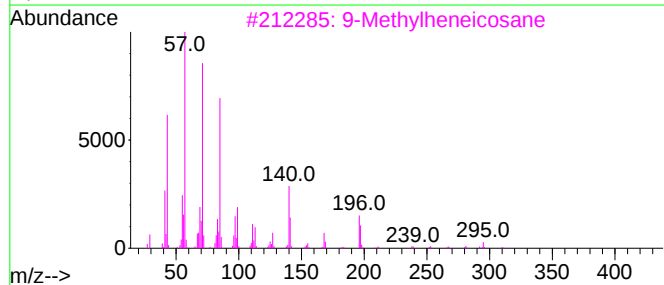
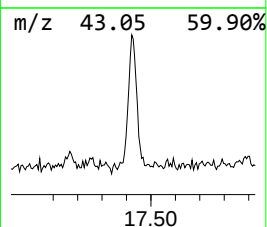
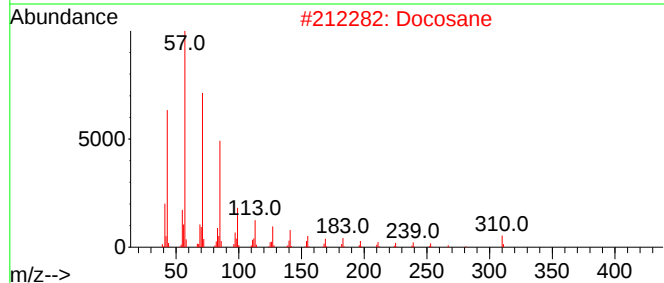
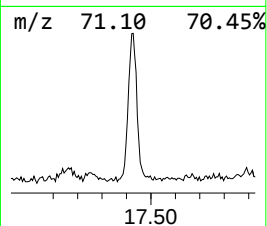
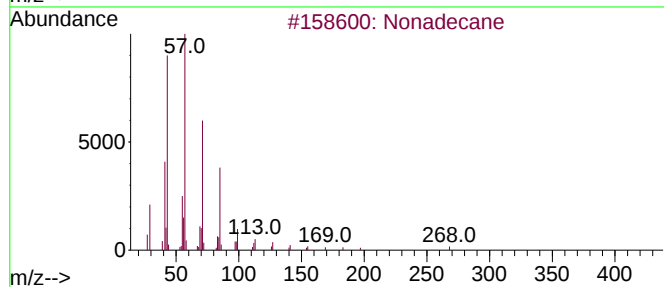
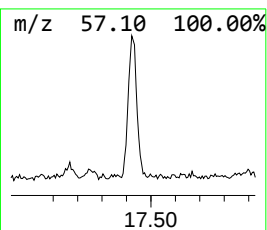
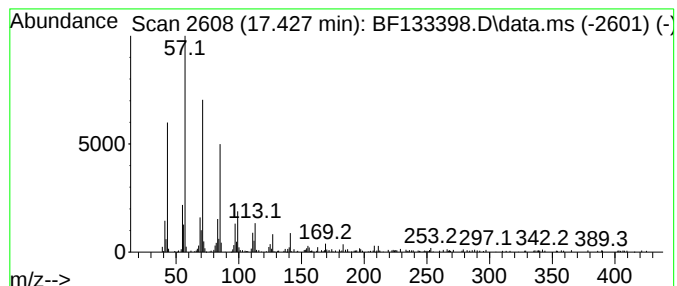
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.427	3.79 ng	337549	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Docosane	310	C22H46	000629-97-0	93
3			9-Methylheneicosane	310	C22H46	070475-51-3	93
4			Hexatriacontane	507	C36H74	000630-06-8	91
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051623\
Data File : BF133398.D
Acq On : 16 May 2023 12:49
Operator : CG\JU
Sample : PB152835BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152835BL

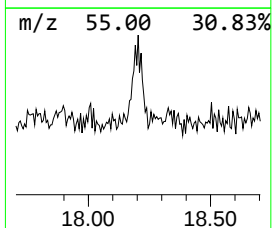
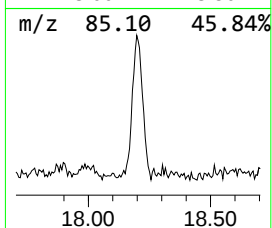
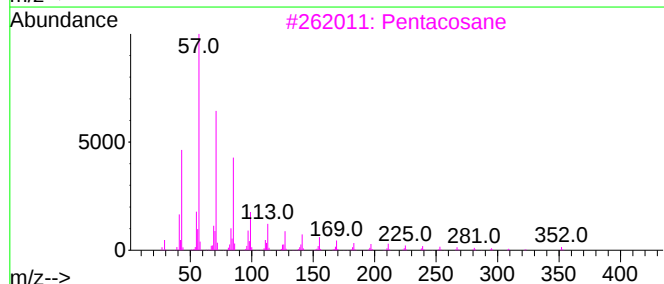
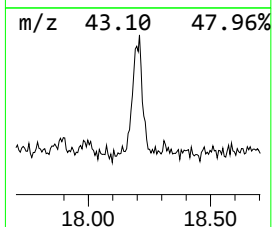
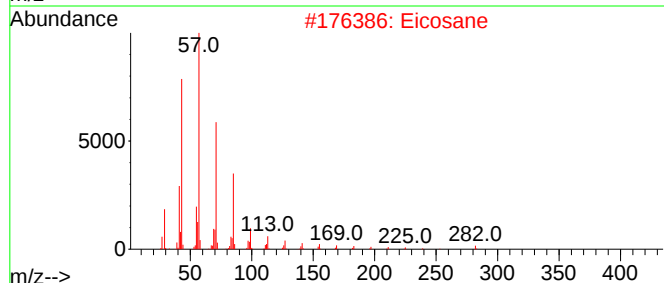
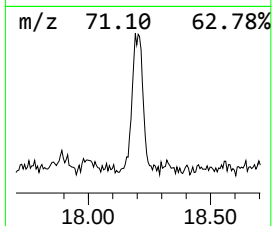
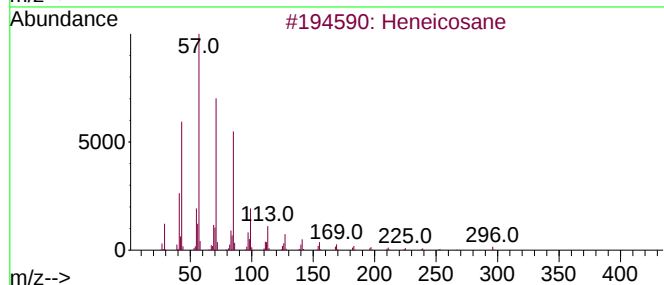
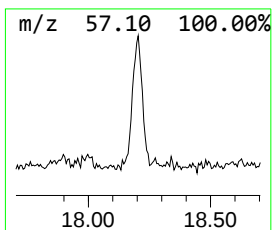
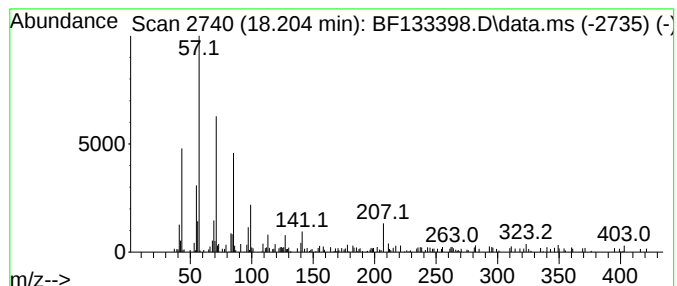
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.204	2.53 ng	225174	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	86
2			Eicosane	282	C20H42	000112-95-8	83
3			Pentacosane	352	C25H52	000629-99-2	72
4			Docosane	310	C22H46	000629-97-0	70
5			6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051623\
Data File : BF133398.D
Acq On : 16 May 2023 12:49
Operator : CG\JU
Sample : PB152835BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB152835BL

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
2-Pentanone, 4-...	4.928	45.6	ng	4139880	1	6.722	1814520	20.0
Tetracosane	14.651	3.0	ng	269278	6	15.304	1781230	20.0
Tricosane	14.974	4.2	ng	370065	6	15.304	1781230	20.0
Heptacosane	15.745	4.7	ng	420017	6	15.304	1781230	20.0
Octadecane, 2-m...	16.215	5.5	ng	491395	6	15.304	1781230	20.0
Hexatriacontane	16.774	3.9	ng	348033	6	15.304	1781230	20.0
Nonadecane	17.427	3.8	ng	337549	6	15.304	1781230	20.0
Heneicosane	18.204	2.5	ng	225174	6	15.304	1781230	20.0