

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
 Data File : BF137078.D
 Acq On : 16 Jan 2024 14:38
 Operator : CG\JU
 Sample : PB158434BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB158434BL

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	502	506	517	rBV2	41168	73648	2.34%	0.395%
2	5.446	566	571	574	rBV	2415514	2442552	77.63%	13.086%
3	6.446	735	741	744	rBV	2233202	2438544	77.50%	13.064%
4	6.787	795	799	802	rBV	532167	448693	14.26%	2.404%
5	7.351	889	895	898	rBV	1446170	1678301	53.34%	8.991%
6	8.057	1011	1015	1019	rBV	629997	595066	18.91%	3.188%
7	9.145	1193	1200	1202	rBV	3020170	3146353	100.00%	16.856%
8	9.816	1310	1314	1318	rBV	740263	677062	21.52%	3.627%
9	10.622	1446	1451	1454	rBV	1832400	1726137	54.86%	9.247%
10	11.316	1565	1569	1572	rBV	808392	707364	22.48%	3.790%
11	12.916	1835	1841	1844	rBV	2911012	3031060	96.34%	16.238%
12	13.974	2017	2021	2028	rVB	547185	487138	15.48%	2.610%
13	14.745	2148	2152	2156	rVB	59938	64407	2.05%	0.345%
14	15.086	2206	2210	2215	rVB	76486	81639	2.59%	0.437%
15	15.468	2270	2275	2283	rVB2	337757	522528	16.61%	2.799%
16	15.927	2347	2353	2358	rVB2	78728	125780	4.00%	0.674%
17	16.445	2436	2441	2447	rVB	74622	136314	4.33%	0.730%
18	17.062	2540	2546	2554	rVB2	52734	114944	3.65%	0.616%
19	17.798	2665	2671	2681	rVB3	39650	105951	3.37%	0.568%
20	18.668	2814	2819	2827	rVB5	23737	62547	1.99%	0.335%

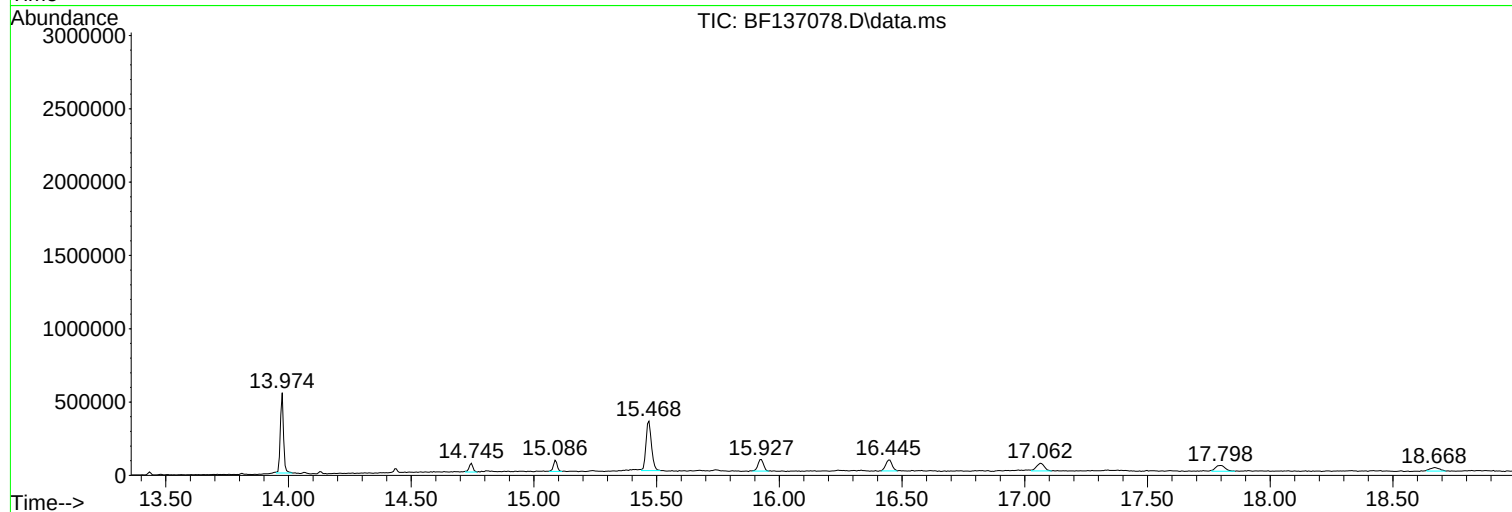
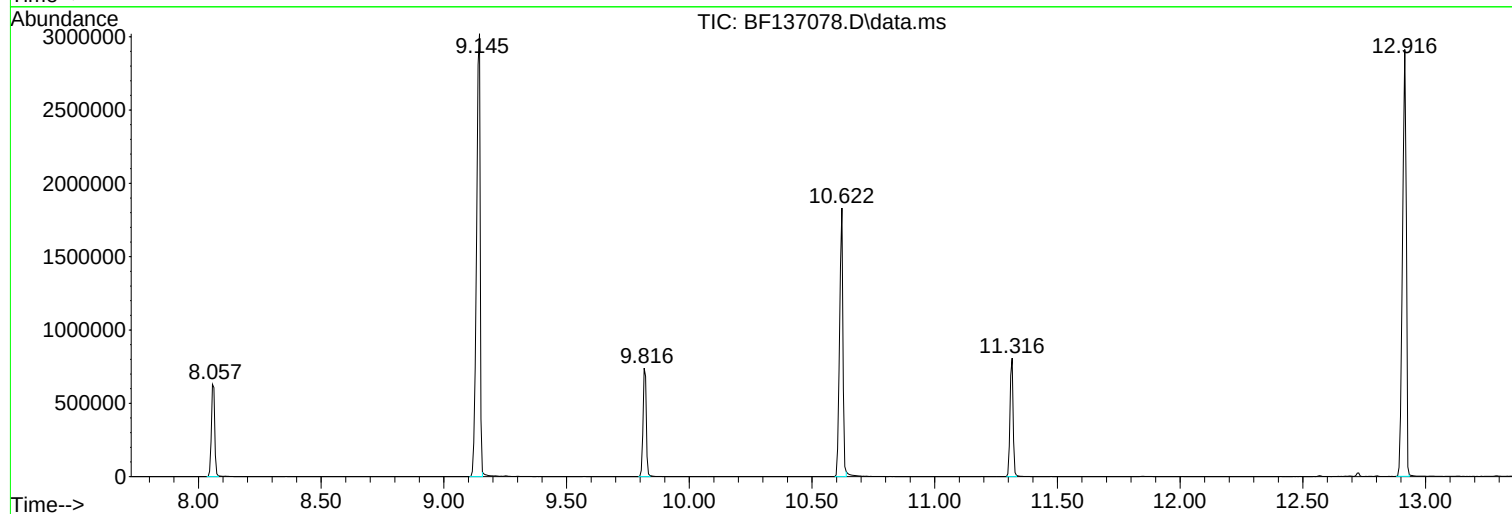
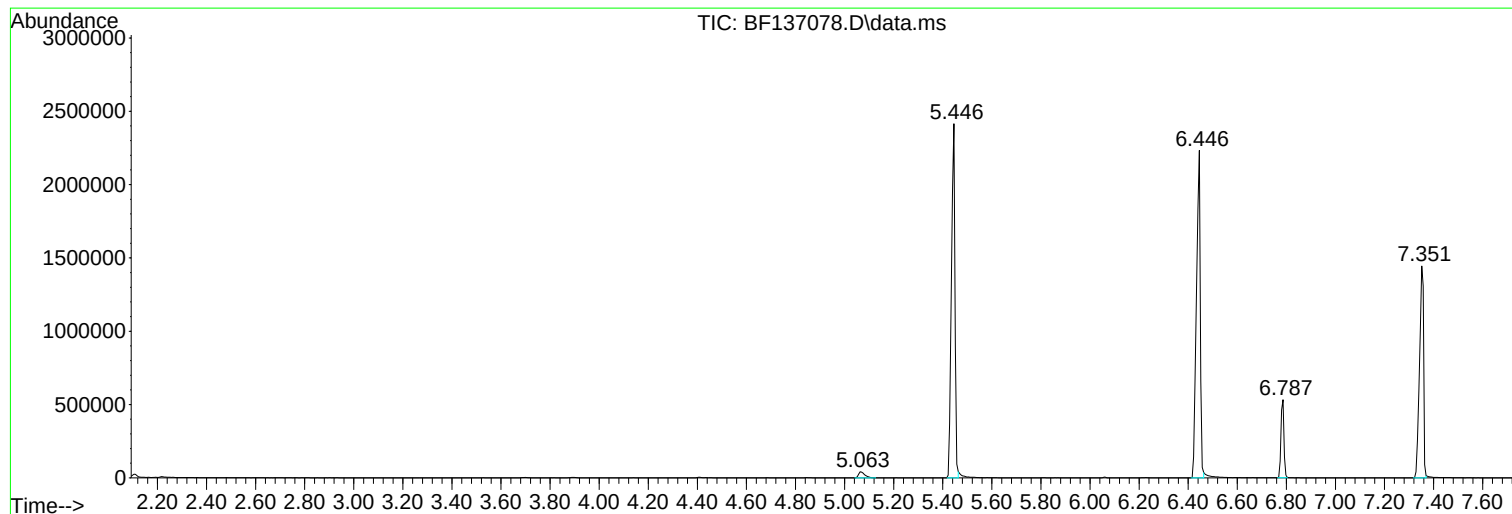
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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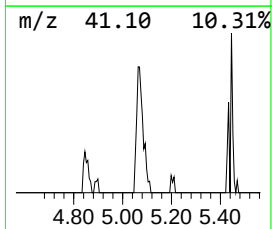
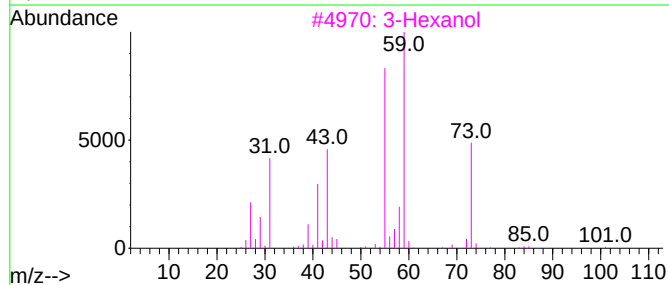
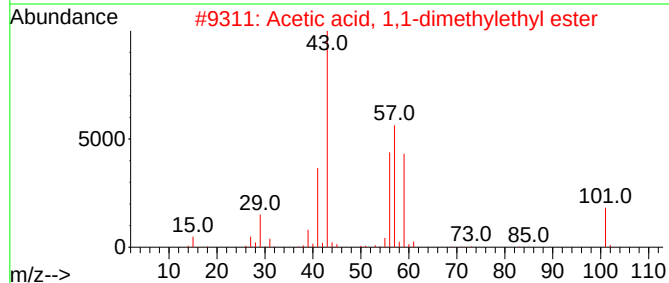
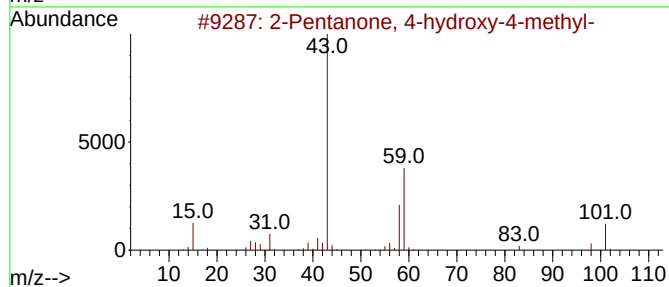
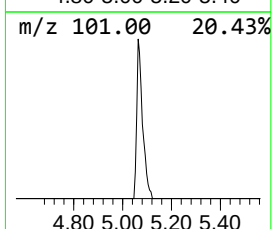
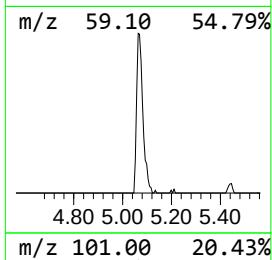
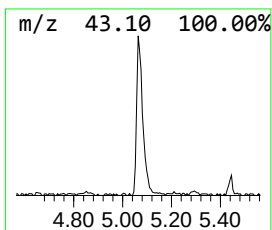
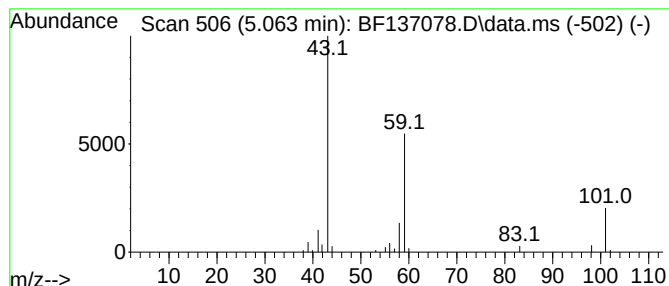
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	3.28 ng	73648	1,4-Dichlorobenzene-d4	6.787

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	3-Hexanol	102	C6H14O	000623-37-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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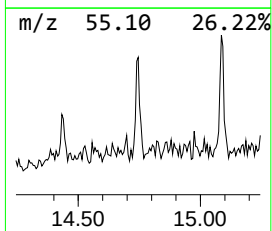
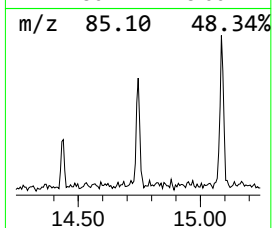
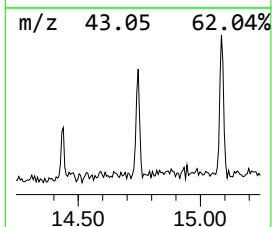
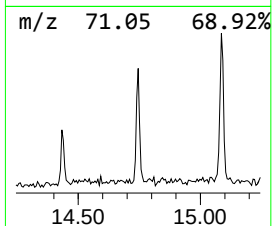
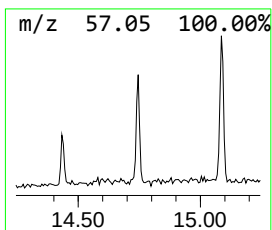
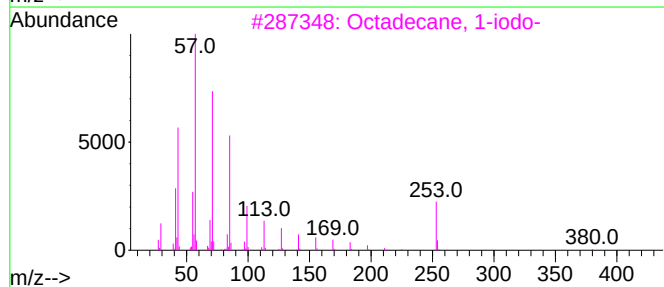
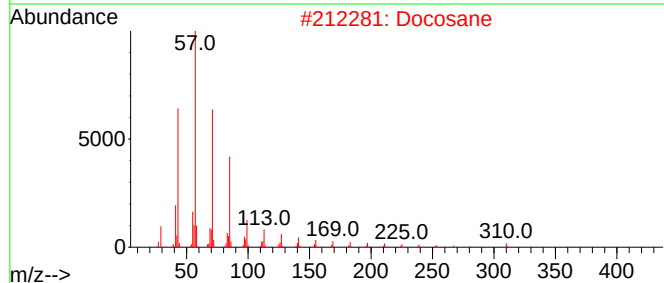
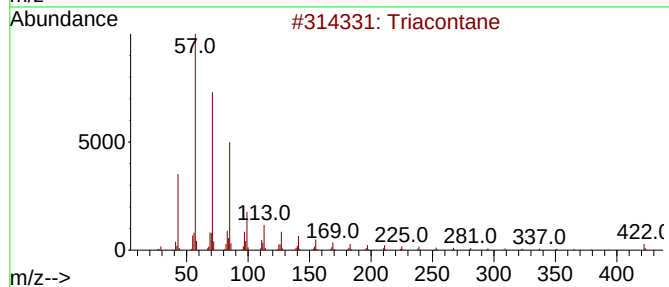
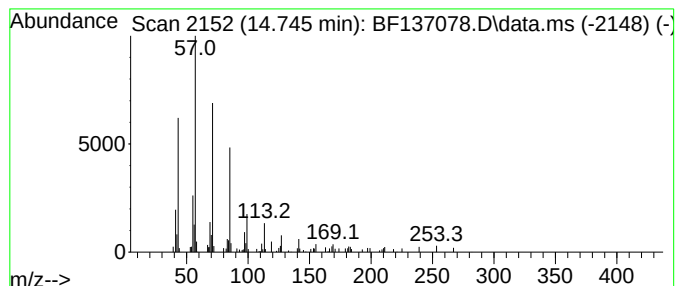
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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Peak Number 2 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.47 ng	64407	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		Docosane	310	C22H46	000629-97-0	91
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86



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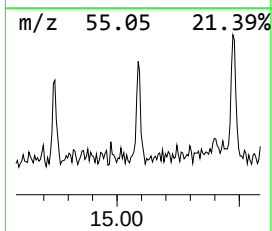
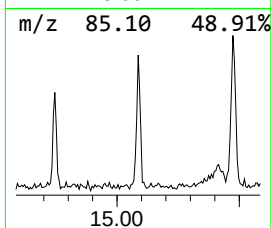
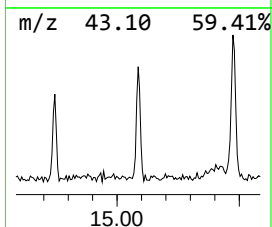
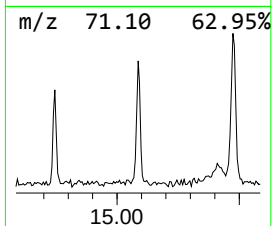
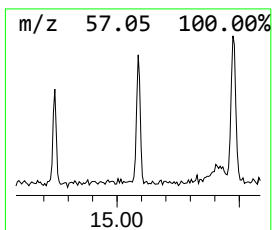
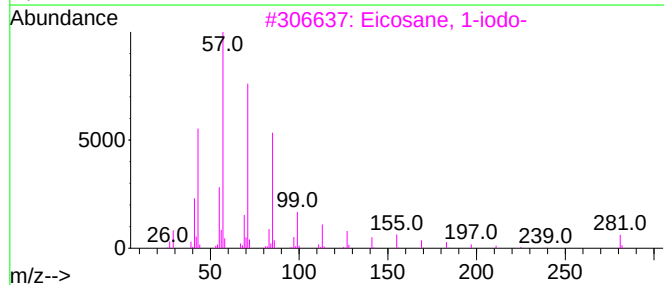
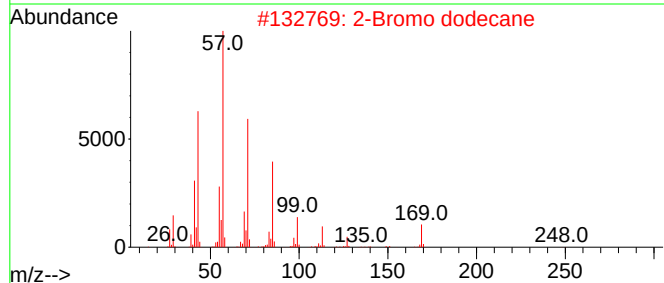
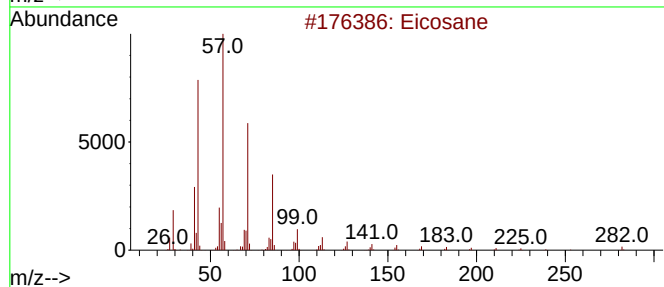
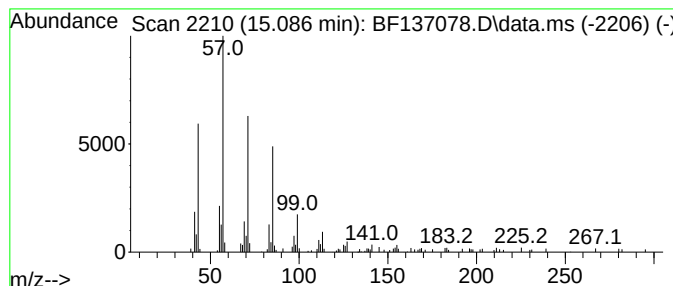
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Peak Number 3 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.12 ng	81639	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	87
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
5			1,3-Propanediol, dodecyl ethyl e...	272	C17H36O2	1000406-35-1	86



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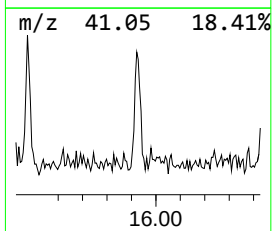
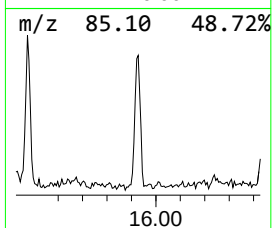
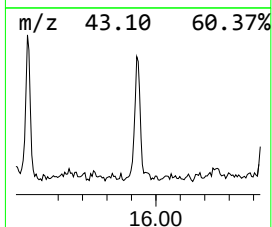
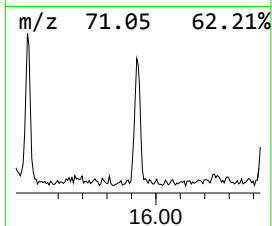
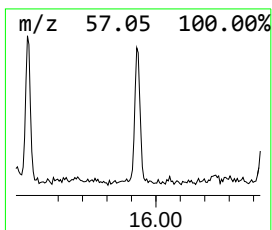
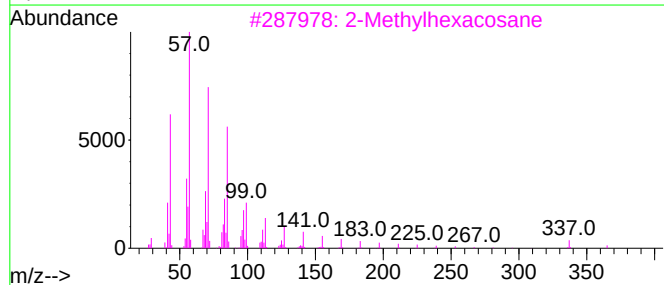
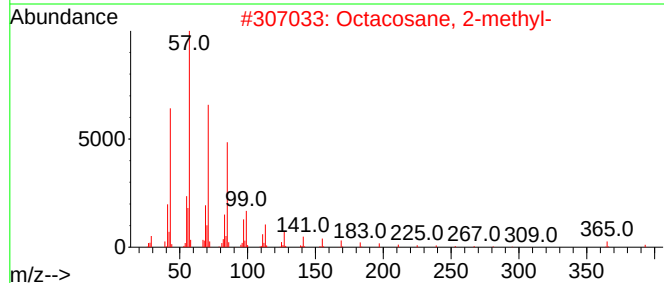
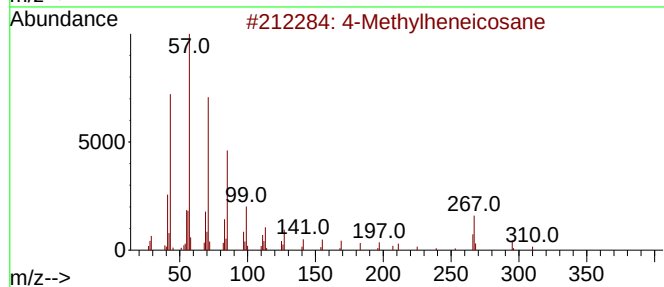
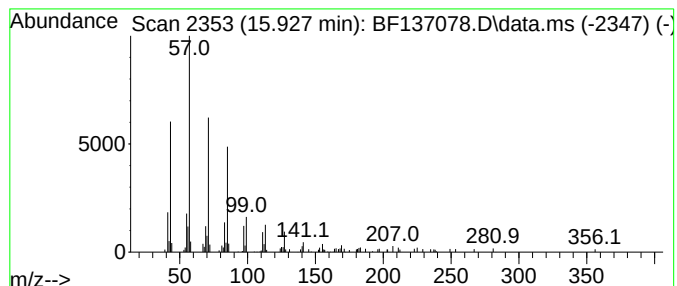
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 4-Methylheneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	4.81 ng	125780	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Methylheneicosane	310	C22H46	025117-29-7	91
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3		2-Methylhexacosane	380	C27H56	001561-02-0	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83



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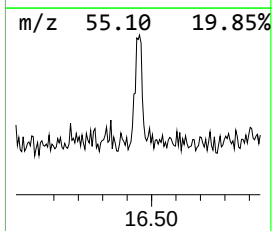
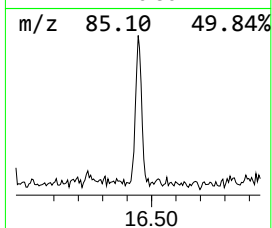
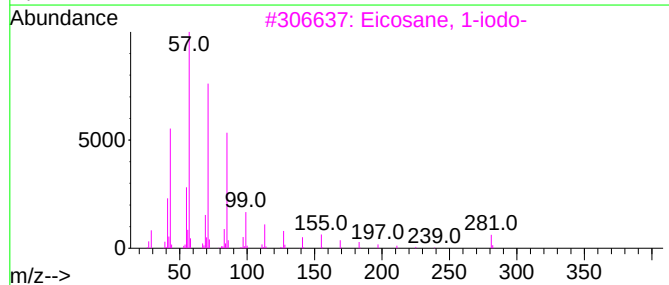
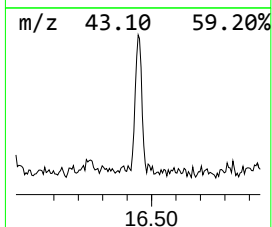
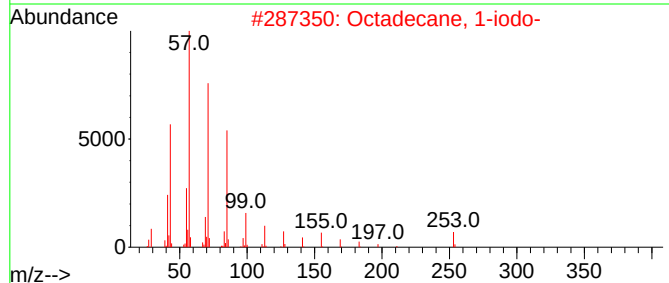
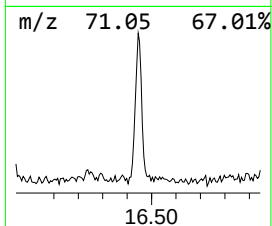
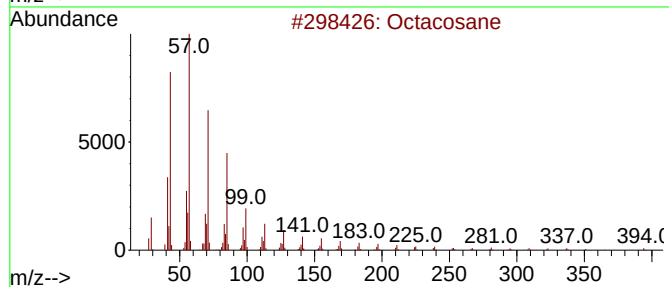
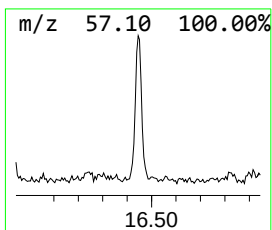
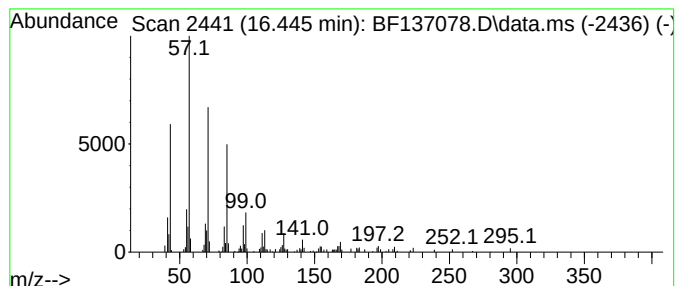
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	5.22 ng	136314	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	86



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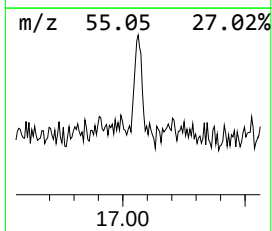
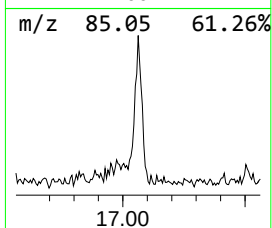
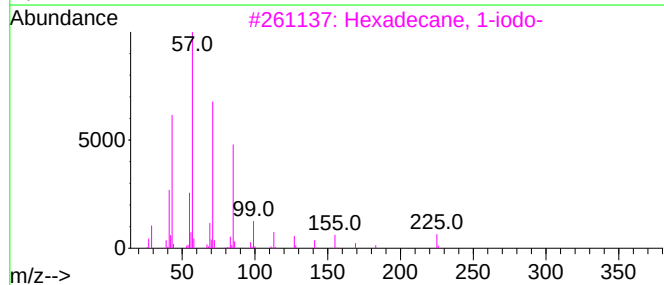
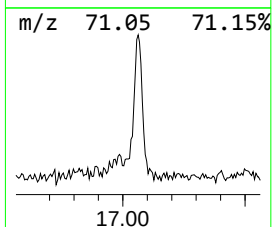
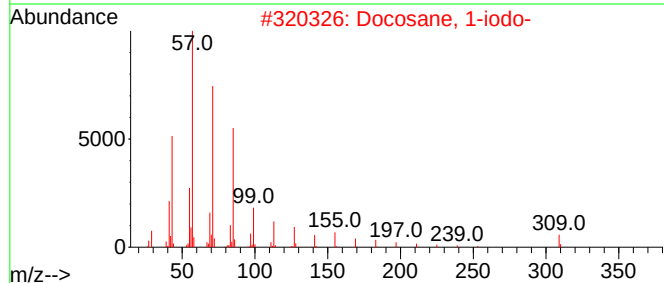
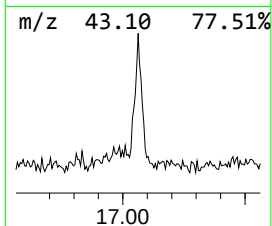
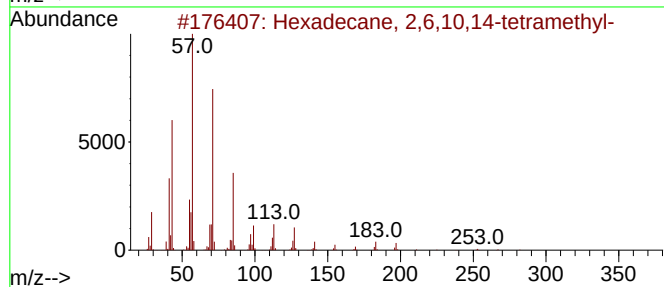
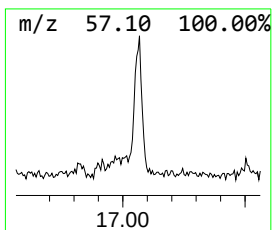
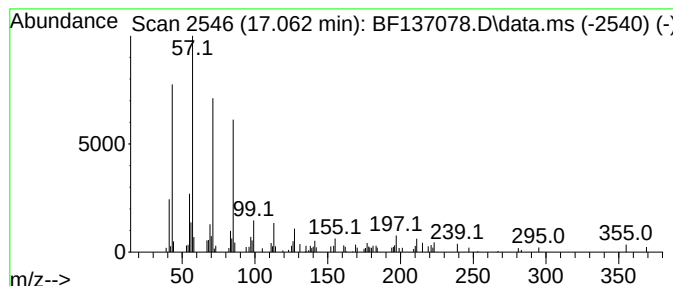
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.063	4.40 ng	114944	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	89
2			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137078.D
Acq On : 16 Jan 2024 14:38
Operator : CG\JU
Sample : PB158434BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158434BL

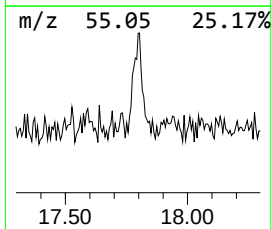
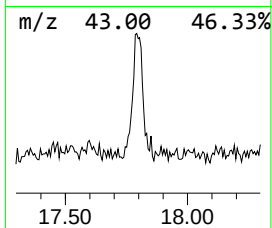
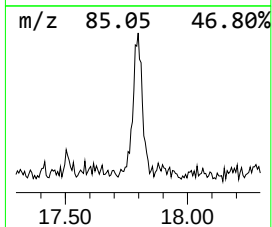
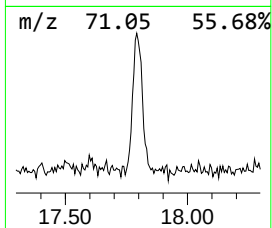
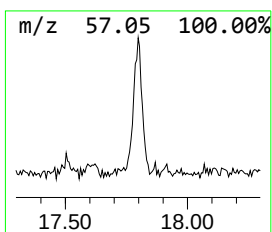
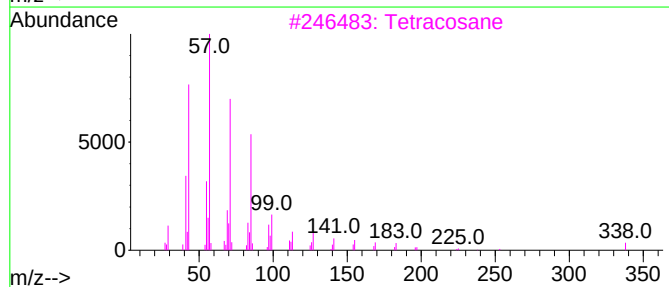
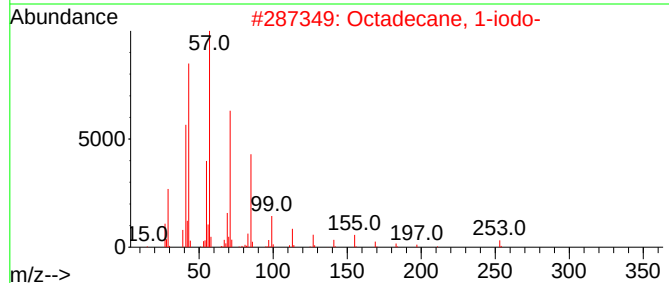
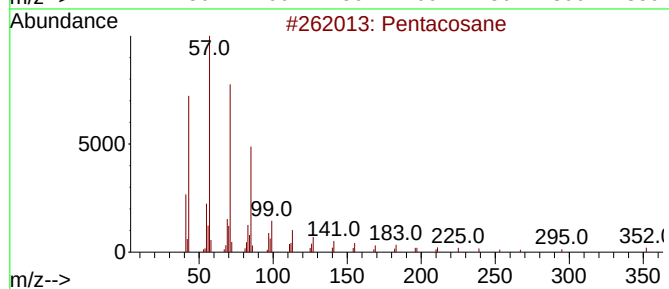
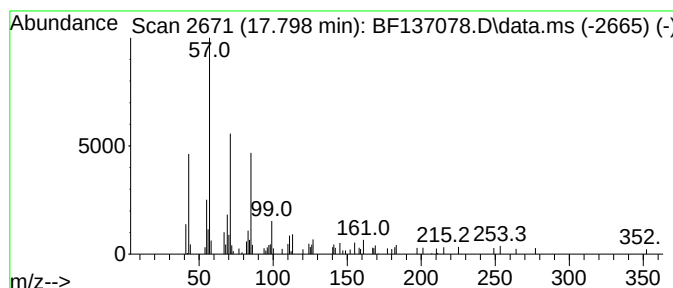
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.798	4.06 ng	105951	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	93
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
3			Tetracosane	338	C24H50	000646-31-1	83
4			Octacosane	394	C28H58	000630-02-4	83
5			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137078.D
Acq On : 16 Jan 2024 14:38
Operator : CG\JU
Sample : PB158434BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158434BL

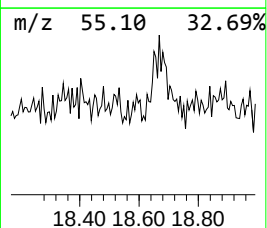
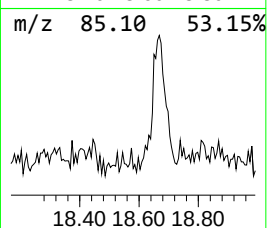
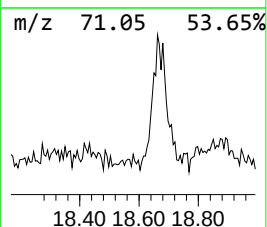
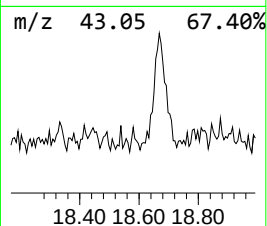
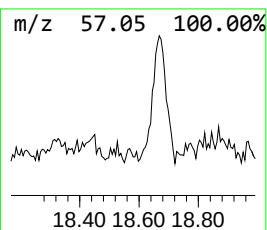
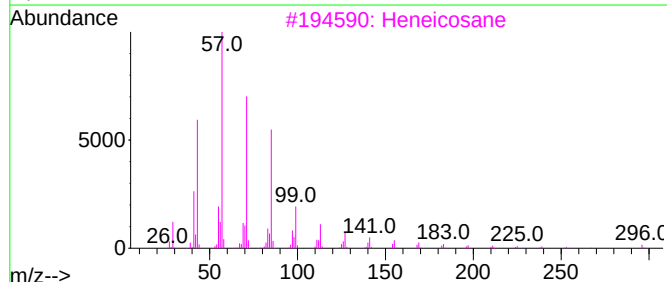
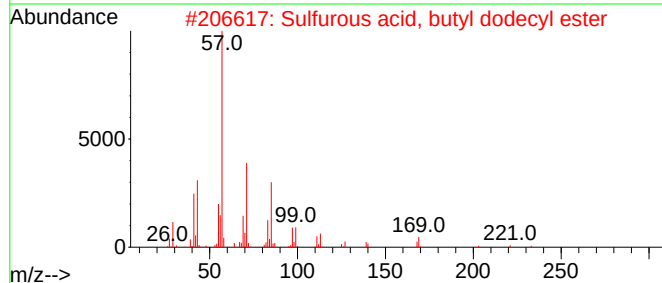
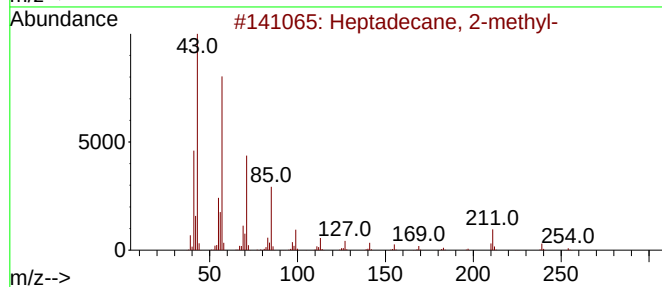
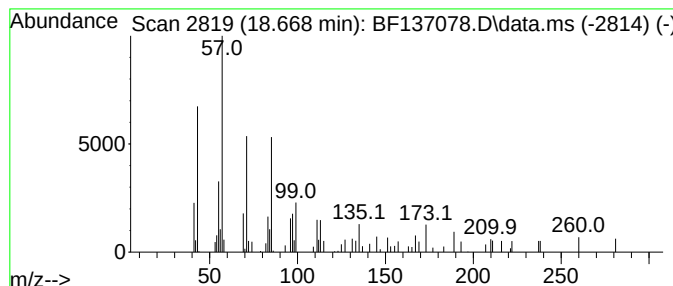
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.668	2.39 ng	62547	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	53
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	52
3			Heneicosane	296	C21H44	000629-94-7	52
4			Heptadecane	240	C17H36	000629-78-7	50
5			Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011624\
Data File : BF137078.D
Acq On : 16 Jan 2024 14:38
Operator : CG\JU
Sample : PB158434BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158434BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.063	3.3	ng	73648	1	6.787	448693	20.0
Triacontane	14.745	2.5	ng	64407	6	15.463	522528	20.0
Eicosane	15.086	3.1	ng	81639	6	15.463	522528	20.0
4-Methylheneico...	15.927	4.8	ng	125780	6	15.463	522528	20.0
Octacosane	16.445	5.2	ng	136314	6	15.463	522528	20.0
Hexadecane, 2,6...	17.063	4.4	ng	114944	6	15.463	522528	20.0
Pentacosane	17.798	4.1	ng	105951	6	15.463	522528	20.0
Heptadecane, 2-...	18.668	2.4	ng	62547	6	15.463	522528	20.0