

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011724\
 Data File : BF137093.D
 Acq On : 17 Jan 2024 15:01
 Operator : CG\JU
 Sample : PB158472BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB158472BL

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: BF137093.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	516	rBV	42430	72417	2.21%	0.384%
2	5.446	566	571	586	rBV	2232446	2466003	75.23%	13.088%
3	6.445	735	741	744	rBV	2061829	2412047	73.58%	12.802%
4	6.781	795	798	802	rBV	528503	433399	13.22%	2.300%
5	7.351	889	895	898	rBV	1486899	1632098	49.79%	8.662%
6	8.057	1011	1015	1019	rBV	628029	580541	17.71%	3.081%
7	9.139	1193	1199	1202	rBV	2941204	3089218	94.24%	16.396%
8	9.816	1310	1314	1327	rBV	805795	672512	20.52%	3.569%
9	10.616	1446	1450	1453	rBV	1711505	1702890	51.95%	9.038%
10	11.310	1564	1568	1572	rBV	841257	713153	21.76%	3.785%
11	12.916	1835	1841	1844	rBV	3099388	3278056	100.00%	17.398%
12	13.974	2017	2021	2031	rVB	539411	550191	16.78%	2.920%
13	14.433	2095	2099	2103	rBV	36911	36049	1.10%	0.191%
14	14.739	2147	2151	2155	rVB	70617	77252	2.36%	0.410%
15	15.086	2206	2210	2216	rVB	92010	99623	3.04%	0.529%
16	15.463	2269	2274	2282	rBV2	360562	543880	16.59%	2.887%
17	15.921	2347	2352	2358	rBV	84496	127919	3.90%	0.679%
18	16.445	2434	2441	2448	rBV2	69736	126225	3.85%	0.670%
19	17.057	2539	2545	2553	rVB3	44016	97403	2.97%	0.517%
20	17.792	2662	2670	2677	rBV4	31102	79567	2.43%	0.422%
21	18.662	2811	2818	2828	rVB6	18063	50707	1.55%	0.269%

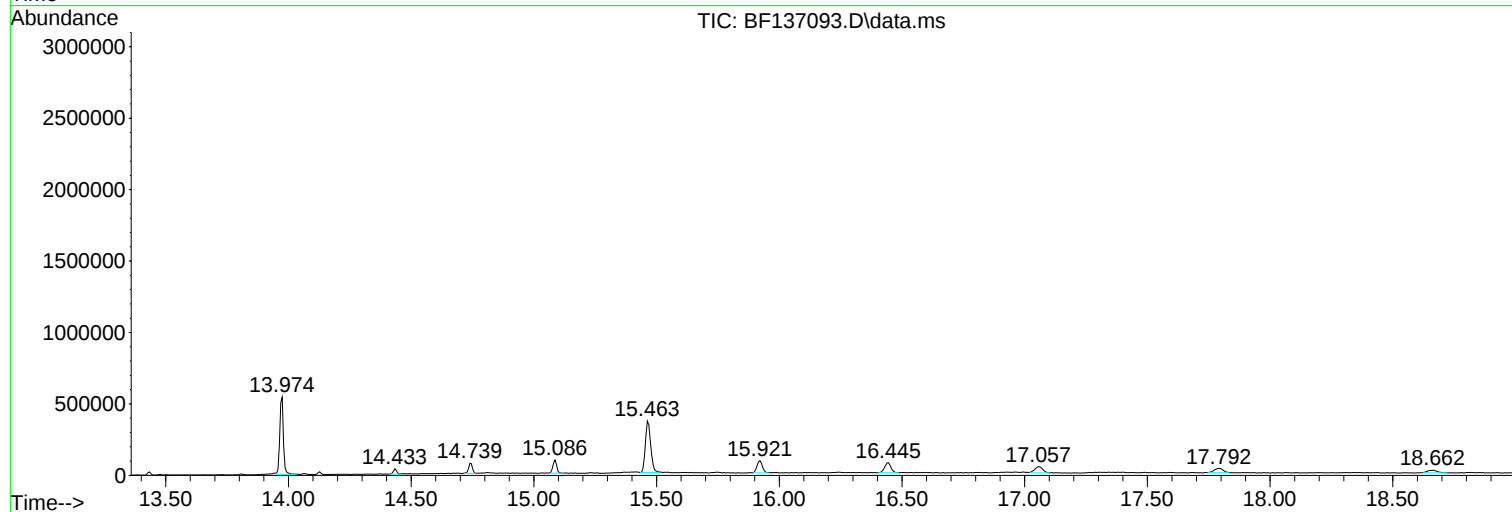
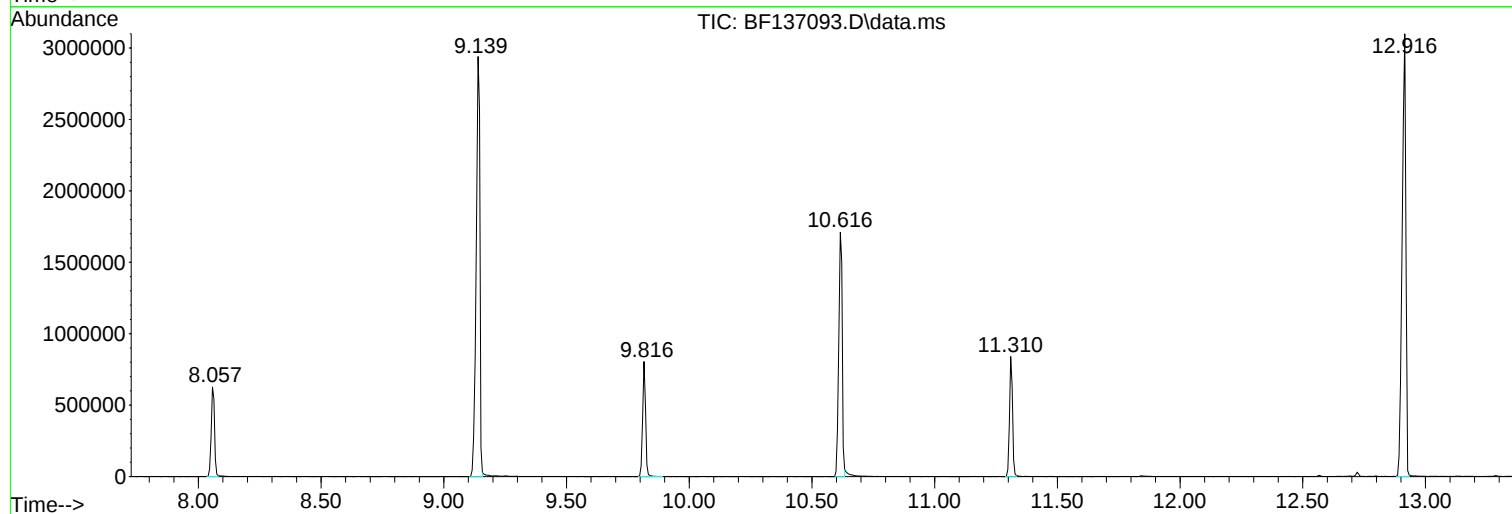
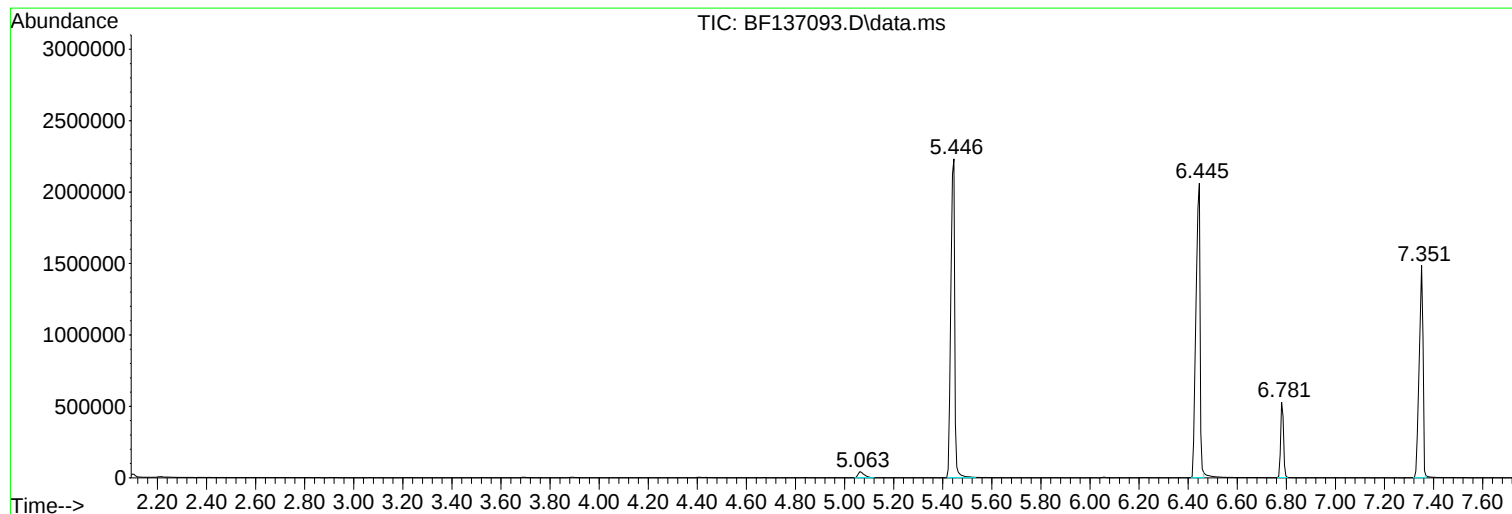
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG\JU
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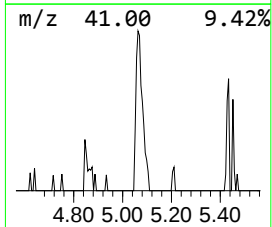
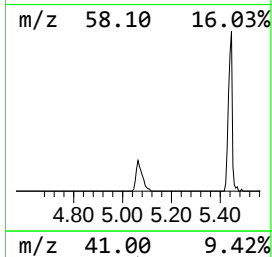
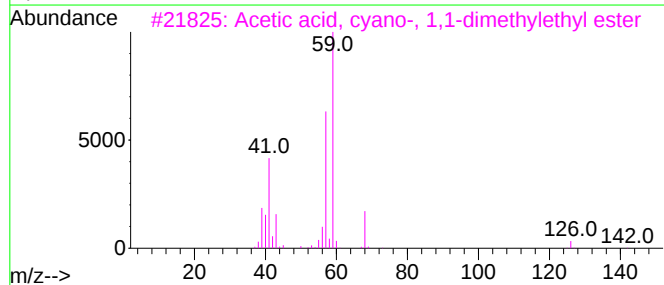
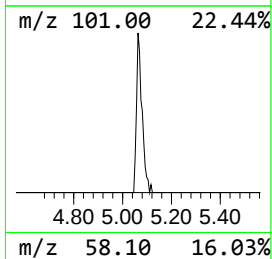
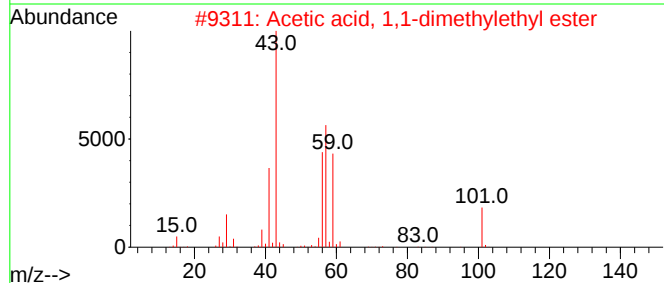
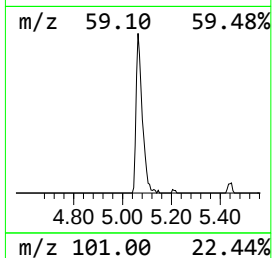
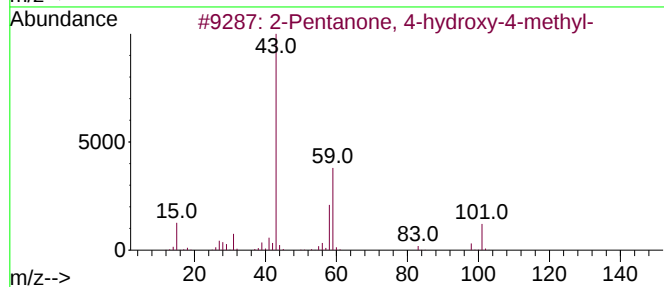
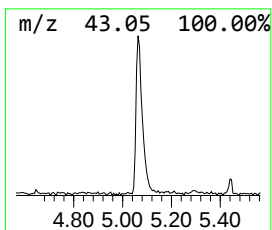
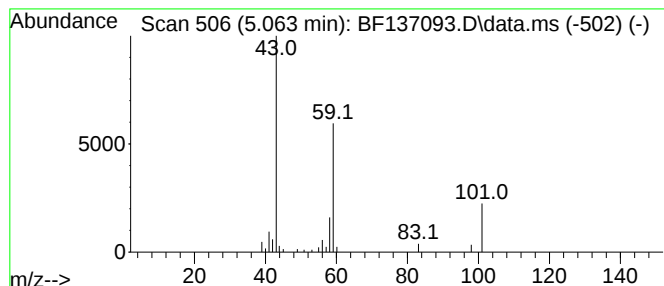
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	3.34 ng	72417	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9		
5	Acetone	58	C3H6O	000067-64-1	9		



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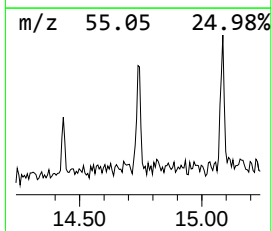
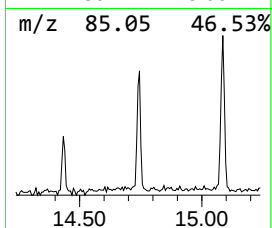
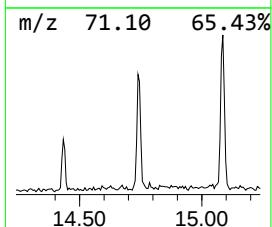
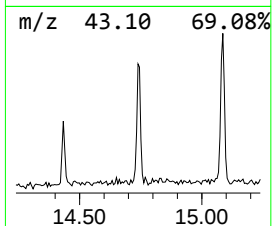
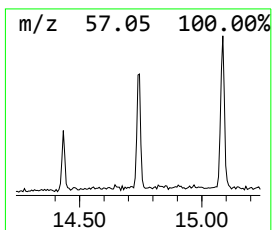
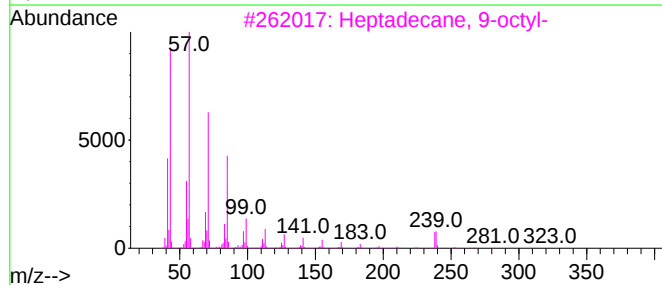
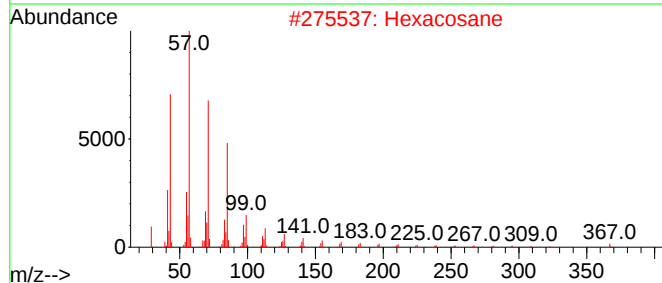
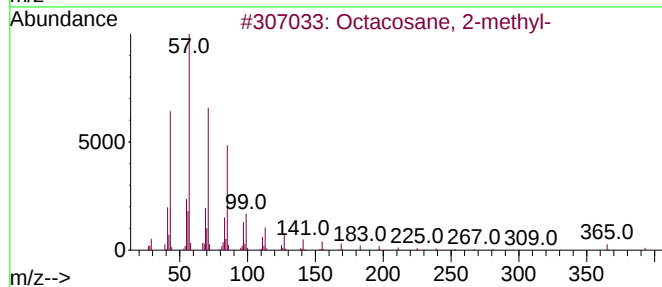
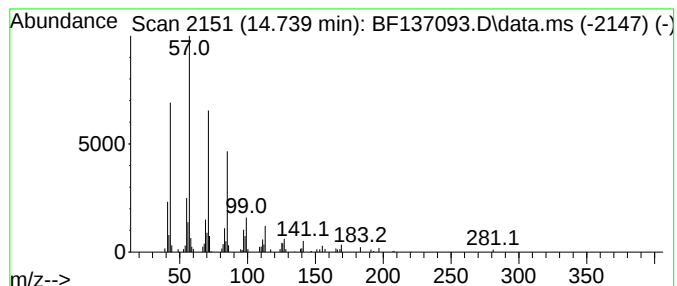
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octacosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	2.84 ng	77252	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



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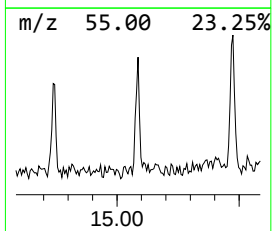
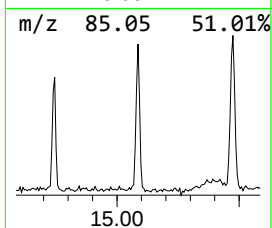
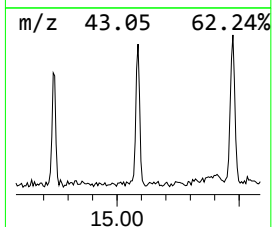
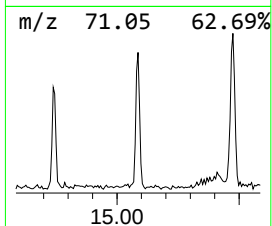
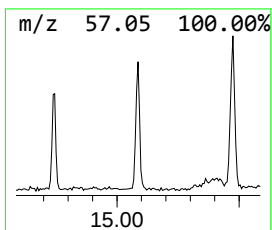
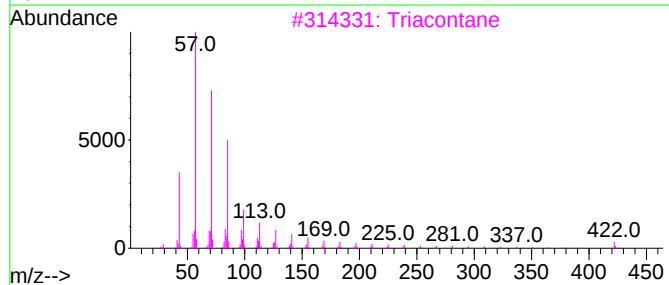
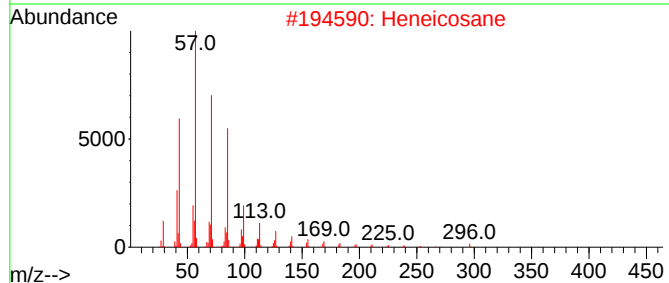
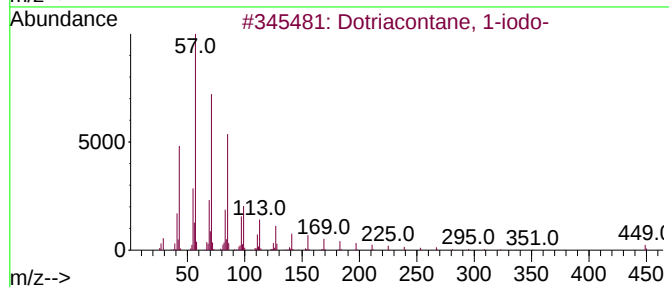
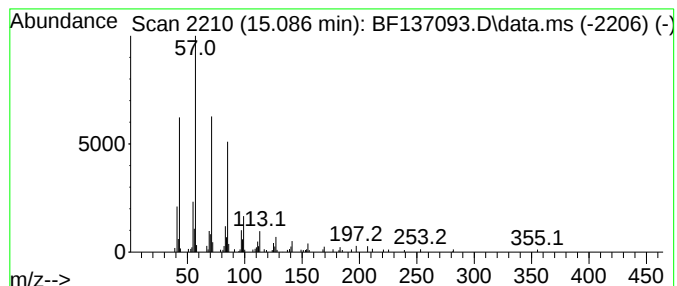
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dotriacontane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.66 ng	99623	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Docosane	310	C22H46	000629-97-0	91
5			Hexadecane	226	C16H34	000544-76-3	86



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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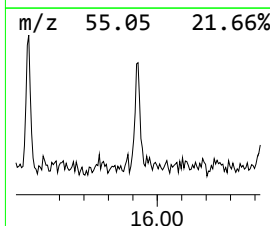
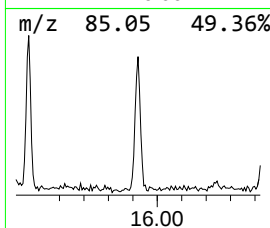
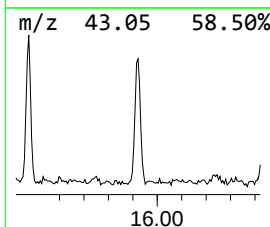
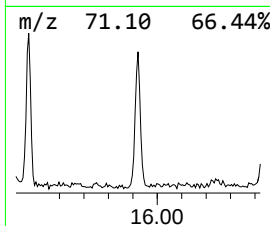
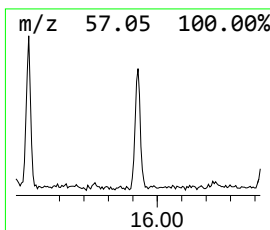
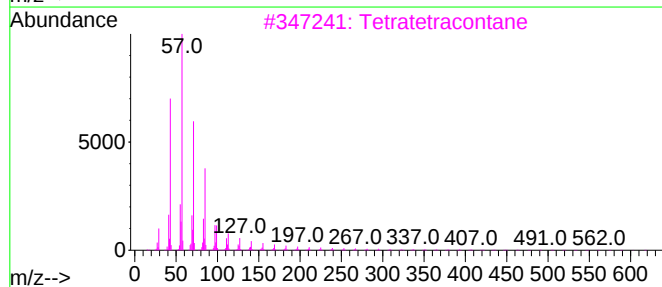
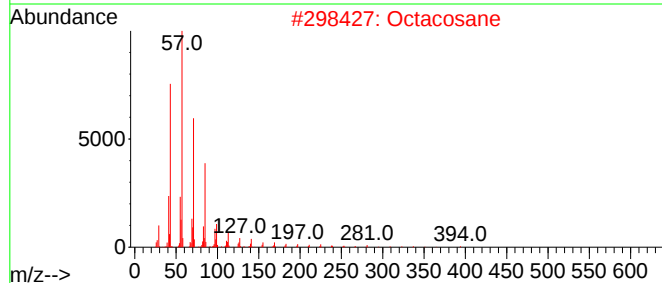
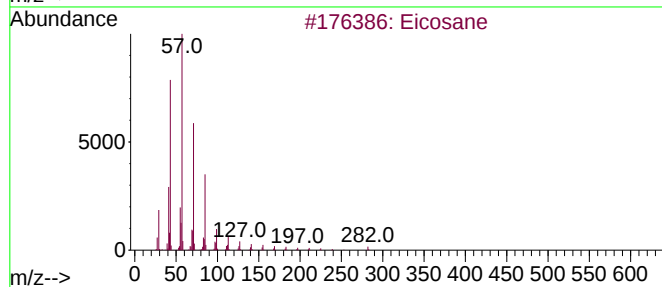
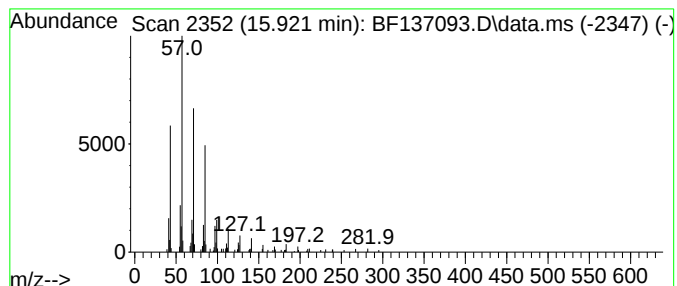
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	4.70 ng	127919	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91



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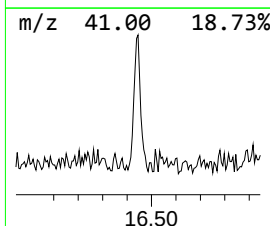
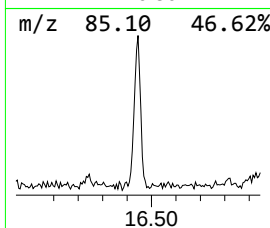
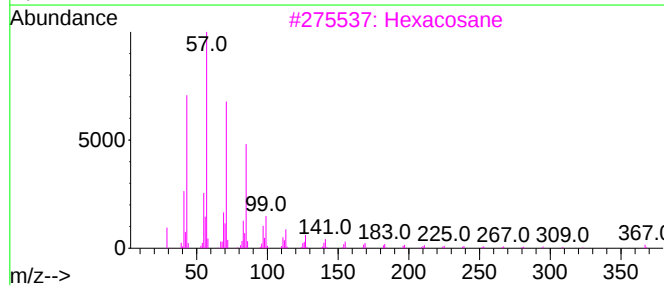
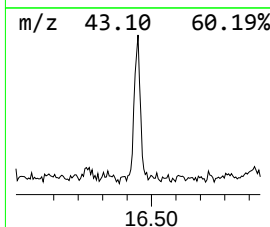
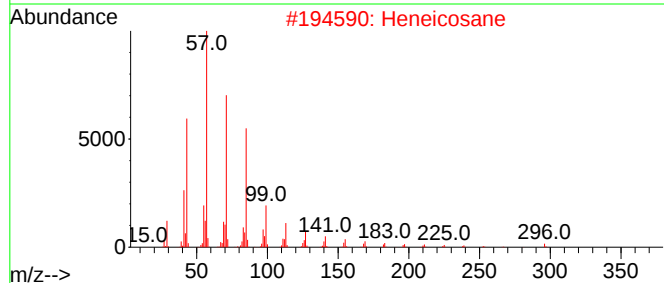
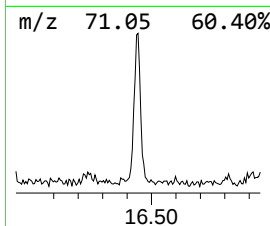
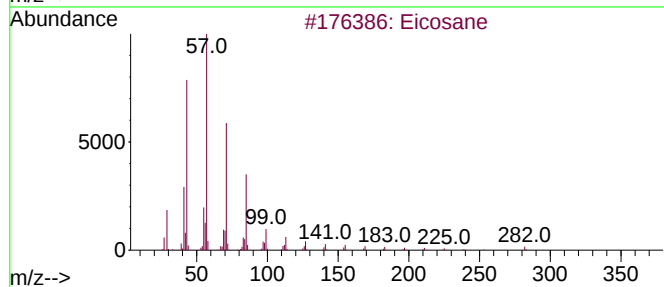
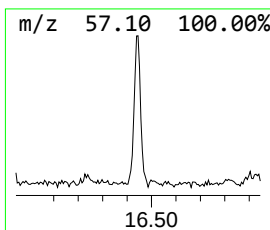
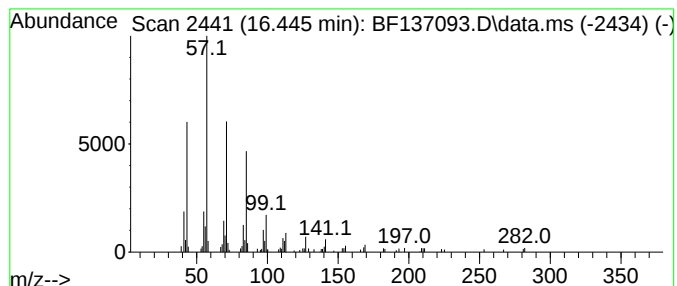
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	4.64 ng	126225	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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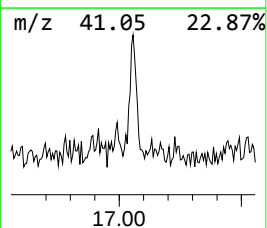
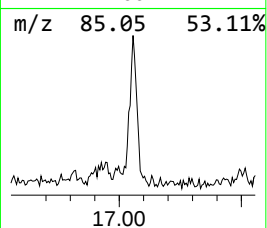
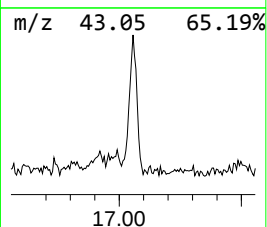
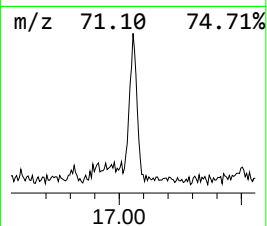
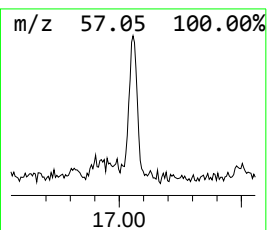
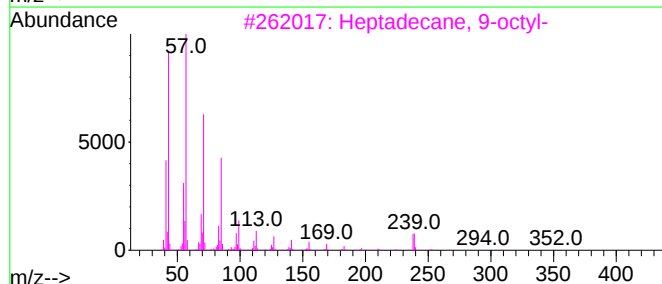
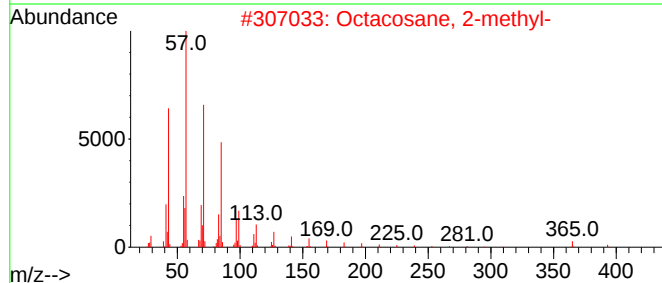
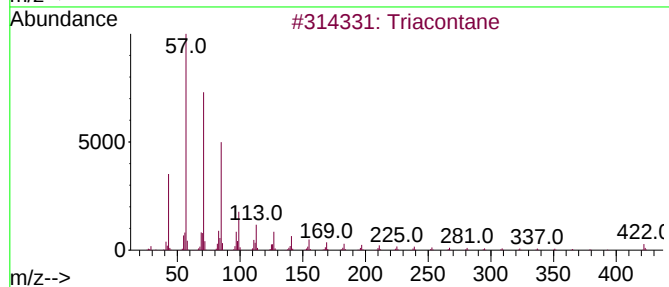
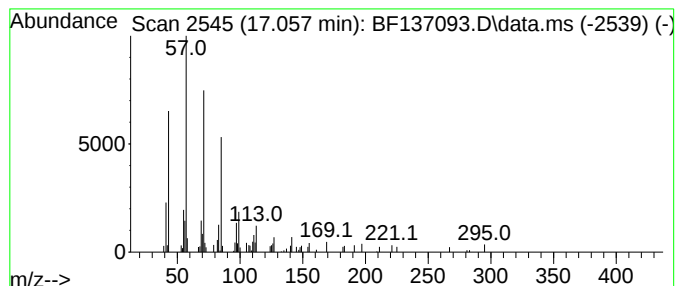
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	3.58 ng	97403	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Docosane	310	C22H46	000629-97-0	91
5			Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011724\
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Acq On : 17 Jan 2024 15:01
Operator : CG\JU
Sample : PB158472BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

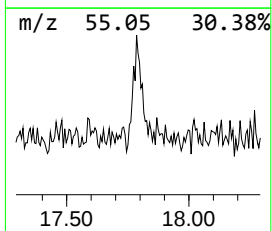
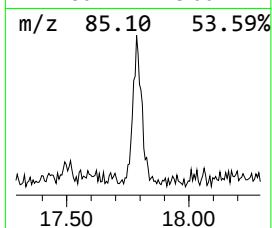
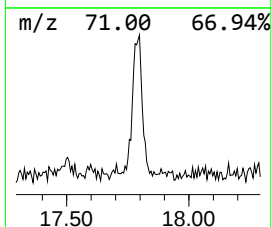
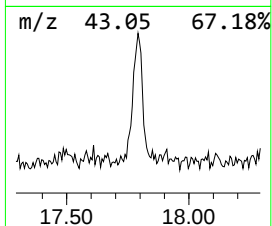
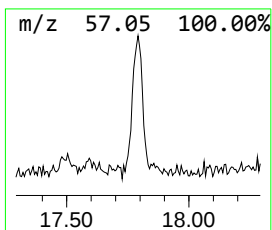
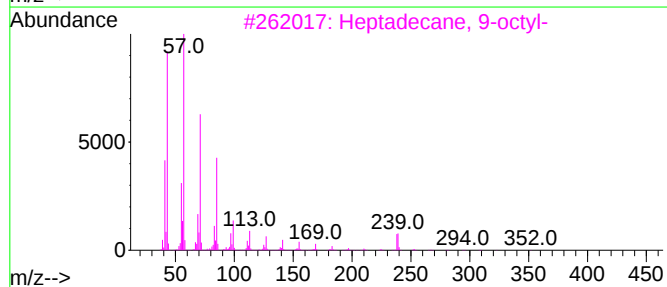
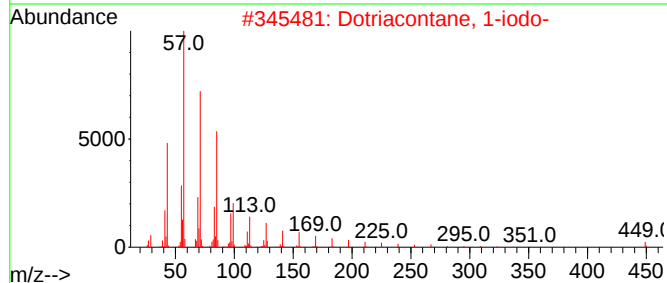
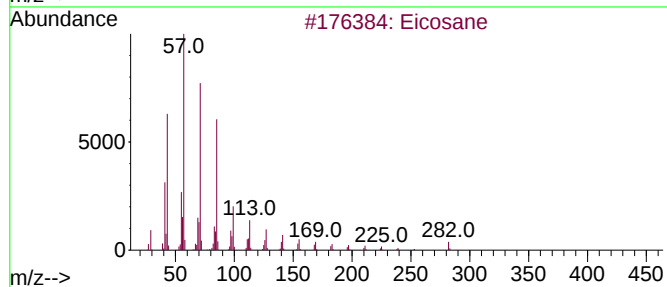
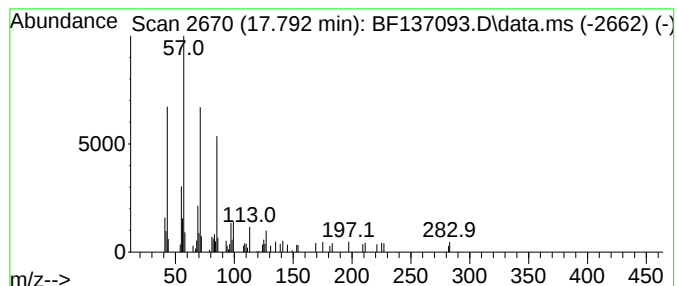
Instrument :
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ClientSampleId :
PB158472BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.792	2.93 ng	79567	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	86
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011724\
Data File : BF137093.D
Acq On : 17 Jan 2024 15:01
Operator : CG\JU
Sample : PB158472BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158472BL

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	72417	1	6.781	433399	20.0
Octacosane, 2-m...	14.739	2.8	ng	77252	6	15.463	543880	20.0
Dotriacontane, ...	15.086	3.7	ng	99623	6	15.463	543880	20.0
Eicosane	15.921	4.7	ng	127919	6	15.463	543880	20.0
Heneicosane	16.445	4.6	ng	126225	6	15.463	543880	20.0
Triacontane	17.057	3.6	ng	97403	6	15.463	543880	20.0
Heptadecane, 9-...	17.792	2.9	ng	79567	6	15.463	543880	20.0