

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
 Data File : BF137790.D
 Acq On : 01 May 2024 14:20
 Operator : CG\JU
 Sample : P2306-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EB-20240429

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-BF043024.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137790.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	27	rVB2	92993	174236	2.29%	0.373%
2	2.428	51	58	64	rBV	992091	1291237	16.94%	2.763%
3	5.681	606	611	614	rBV	4361104	3987009	52.32%	8.532%
4	6.663	773	778	781	rBV	2869953	2774510	36.41%	5.938%
5	7.057	841	845	848	rBV	1580370	1228356	16.12%	2.629%
6	7.622	935	941	944	rBV	3854598	3884578	50.98%	8.313%
7	8.339	1059	1063	1067	rBV	2096348	1793707	23.54%	3.839%
8	9.416	1241	1246	1249	rBV	7902538	7620325	100.00%	16.308%
9	10.104	1359	1363	1366	rVB	2487863	2002690	26.28%	4.286%
10	10.898	1492	1498	1501	rBV	5292383	4970092	65.22%	10.636%
11	11.598	1613	1617	1620	rBV	2447097	1999788	26.24%	4.280%
12	12.098	1697	1702	1708	rBV	336040	381782	5.01%	0.817%
13	12.816	1818	1824	1833	rBV	675934	846384	11.11%	1.811%
14	12.892	1833	1837	1849	rVB	230793	281457	3.69%	0.602%
15	13.192	1883	1888	1891	rBV	7901826	7561627	99.23%	16.182%
16	13.533	1940	1946	1953	rBV	247637	336436	4.41%	0.720%
17	14.104	2039	2043	2051	rVB	331437	420633	5.52%	0.900%
18	14.251	2064	2068	2071	rBV	1483469	1367931	17.95%	2.927%
19	14.598	2122	2127	2131	rBV	416599	506554	6.65%	1.084%
20	15.086	2204	2210	2218	rVB	320940	488176	6.41%	1.045%
21	15.633	2297	2303	2311	rBV	297348	481263	6.32%	1.030%
22	15.821	2329	2335	2344	rBV	964073	1272046	16.69%	2.722%
23	16.251	2401	2408	2415	rBV	190703	391313	5.14%	0.837%
24	16.974	2524	2531	2541	rVB2	138965	305595	4.01%	0.654%
25	17.804	2665	2672	2682	rVB2	80535	208044	2.73%	0.445%
26	18.803	2834	2842	2852	rVB5	48956	151624	1.99%	0.324%

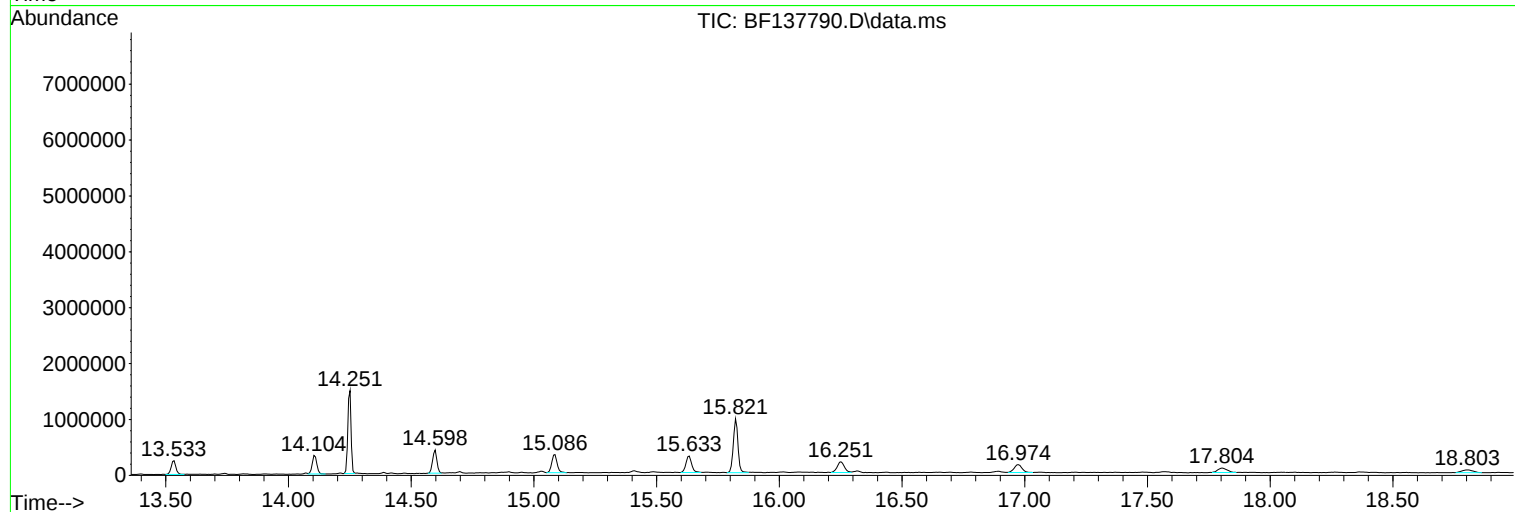
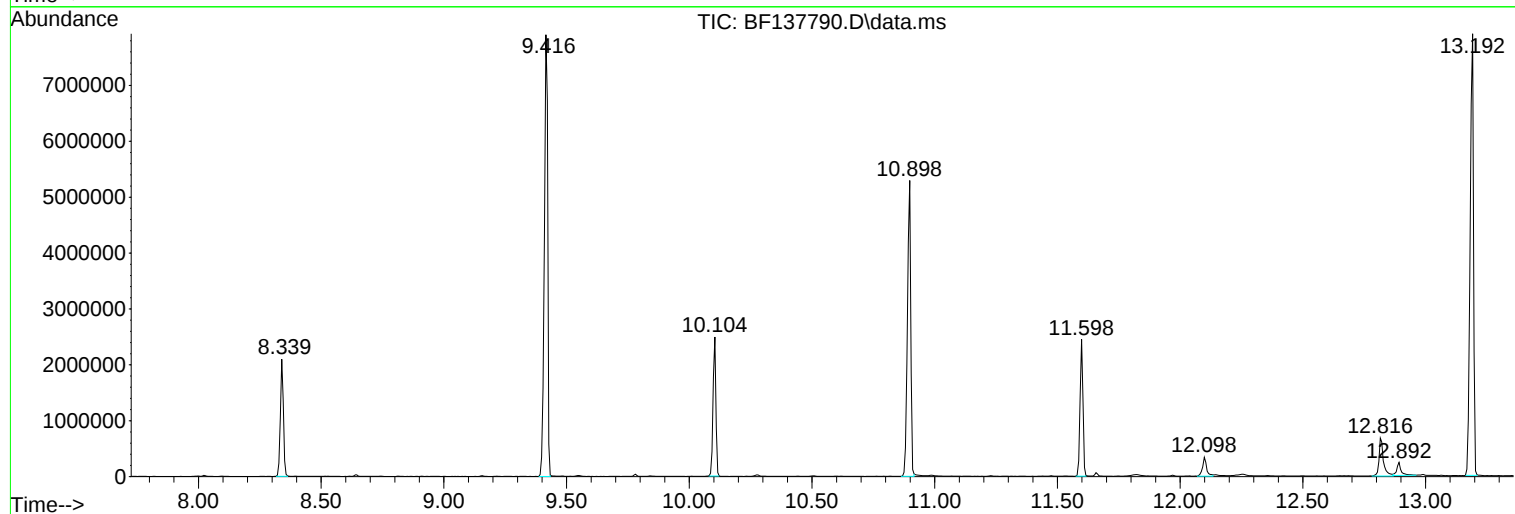
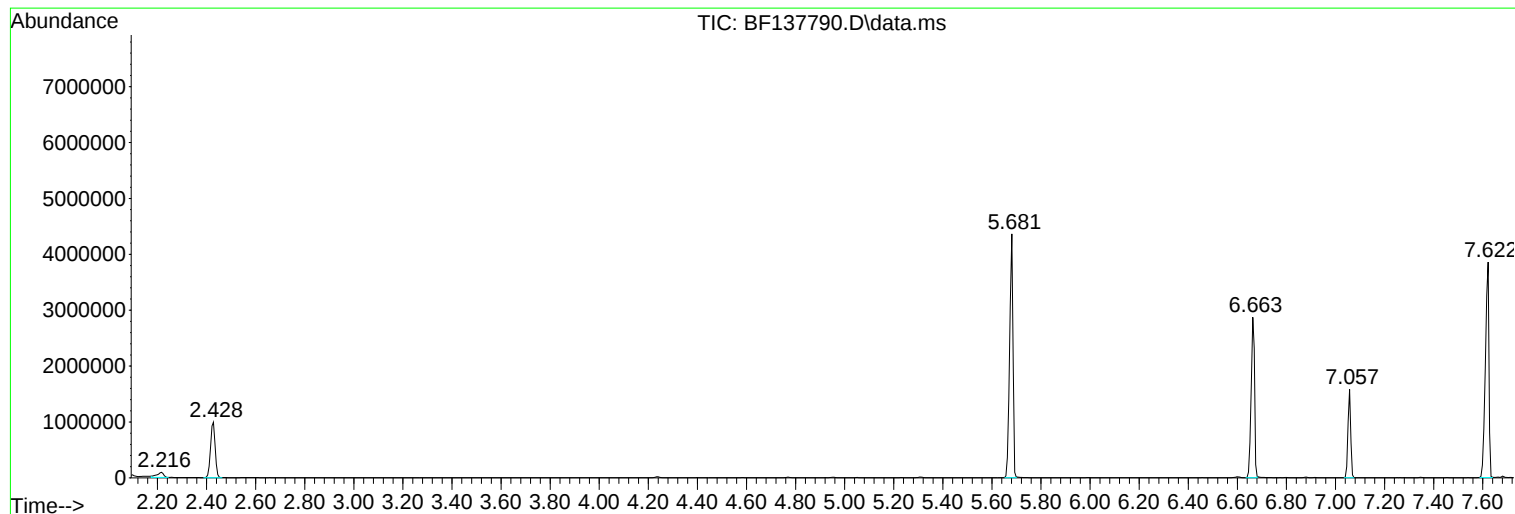
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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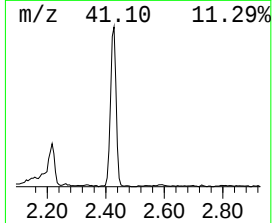
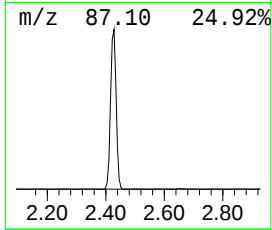
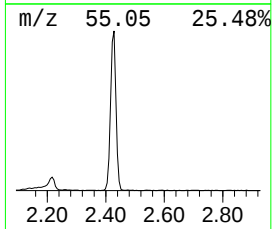
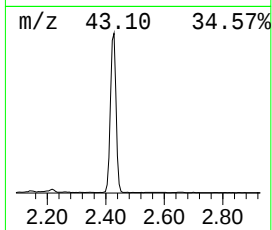
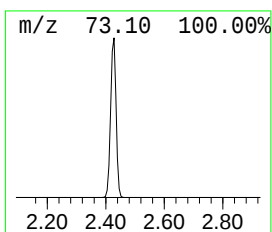
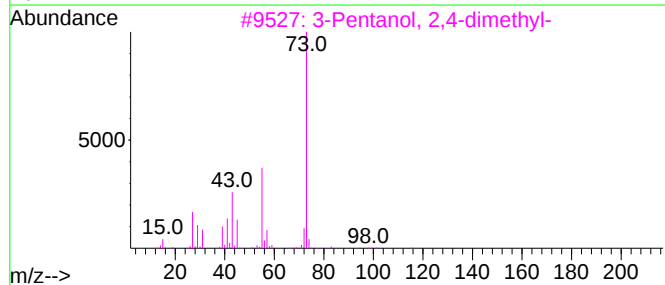
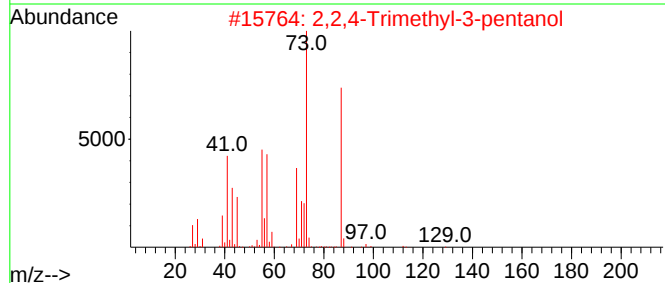
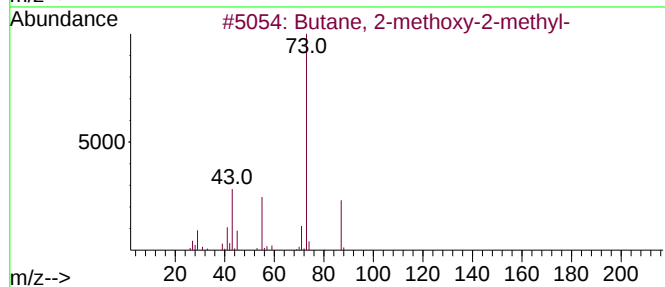
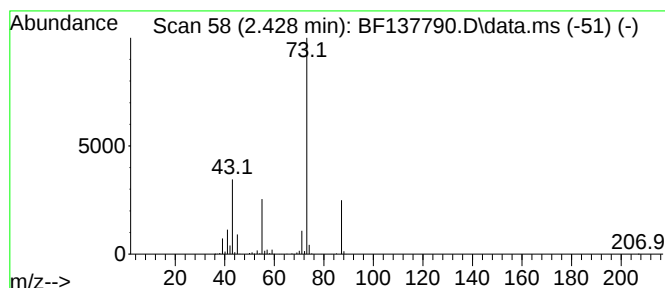
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.428	21.02 ng	1291240	1,4-Dichlorobenzene-d4	7.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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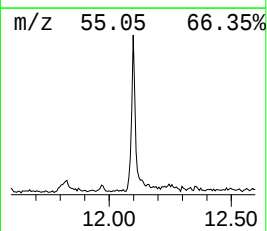
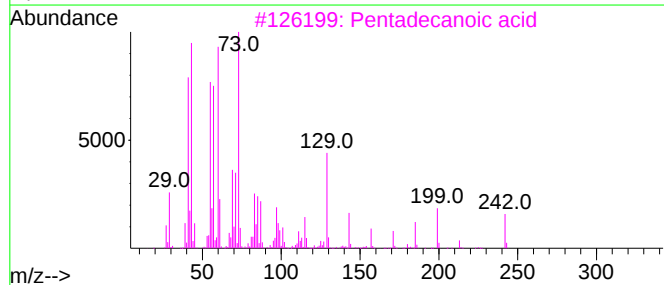
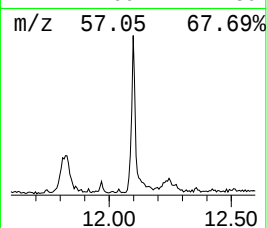
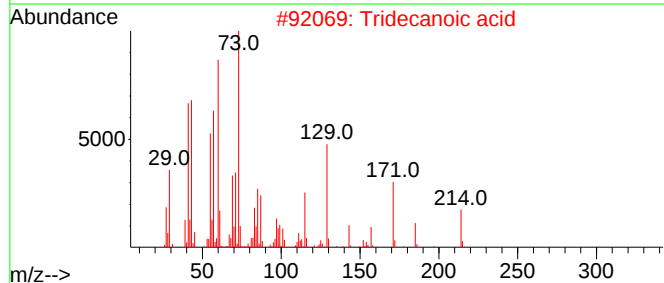
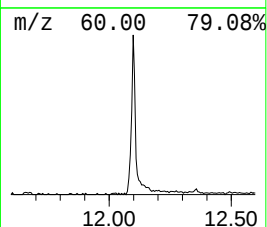
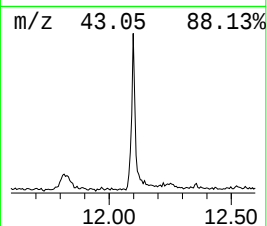
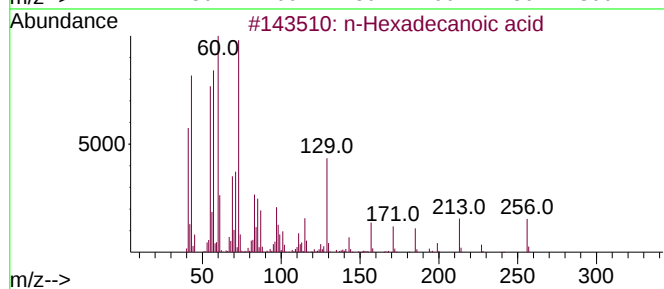
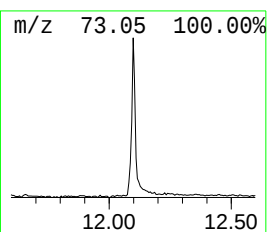
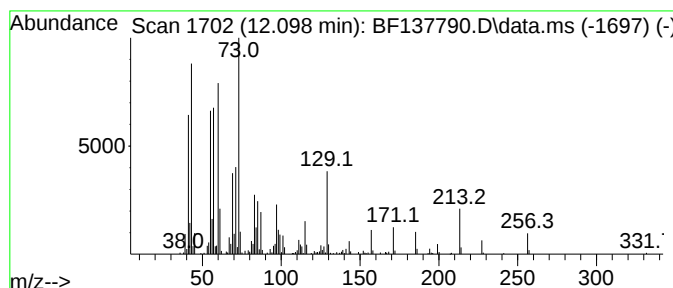
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	3.82 ng	381782	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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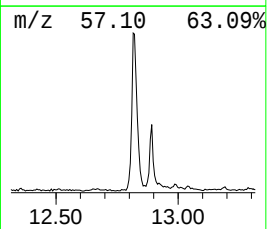
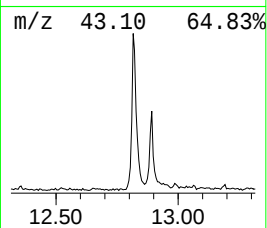
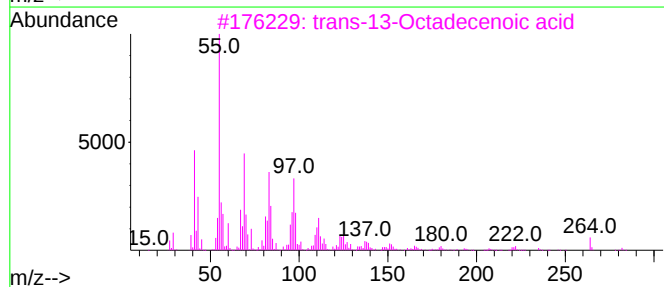
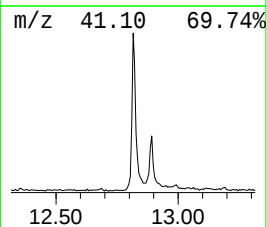
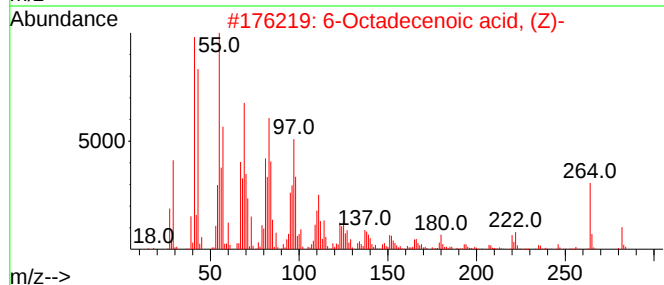
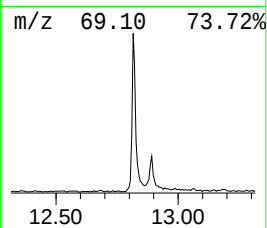
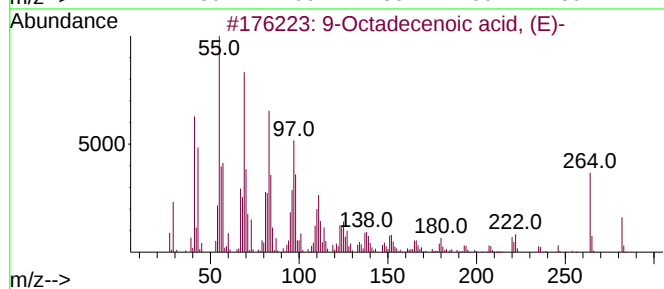
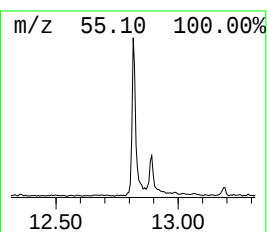
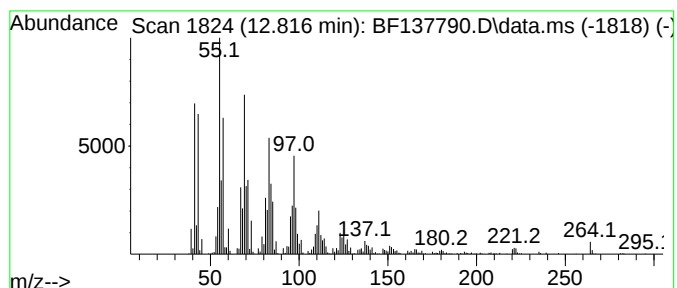
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	8.46 ng	846384	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	98
2			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	96
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
4			9-Octadecenoic acid	282	C18H34O2	002027-47-6	90
5			Oleic Acid	282	C18H34O2	000112-80-1	90



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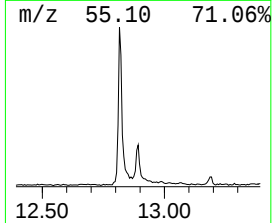
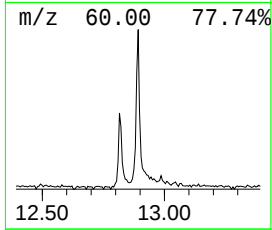
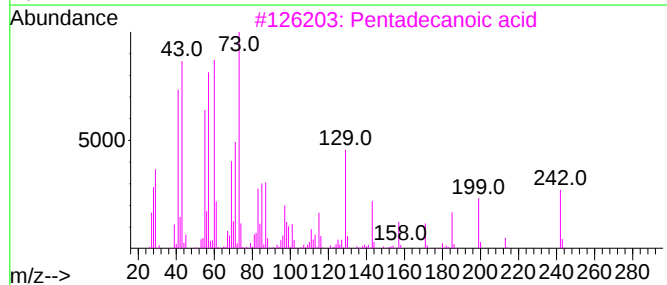
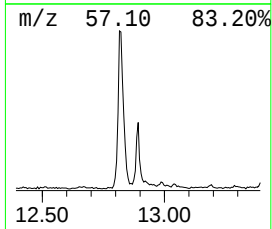
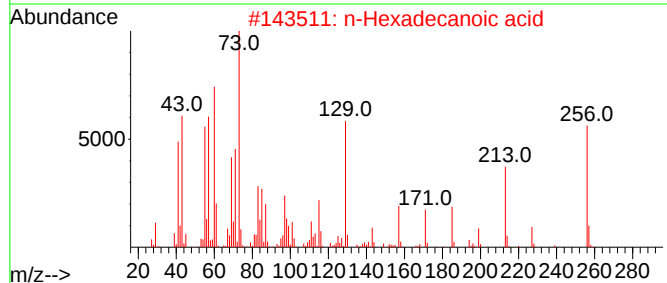
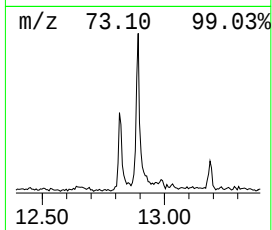
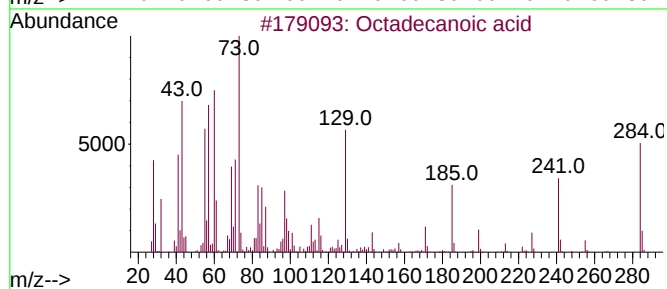
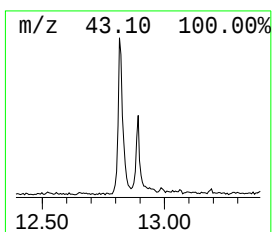
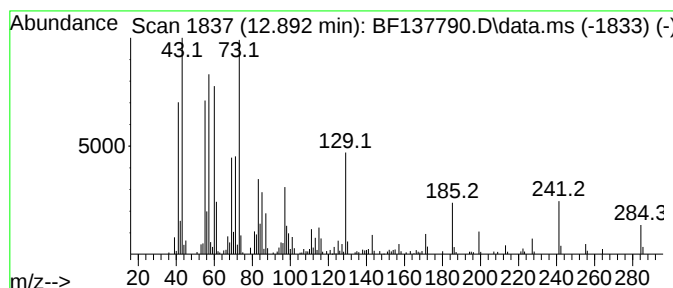
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	2.81 ng	281457	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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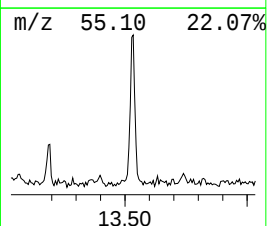
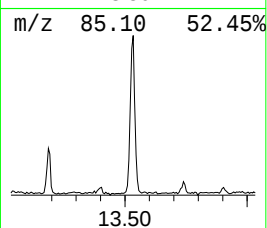
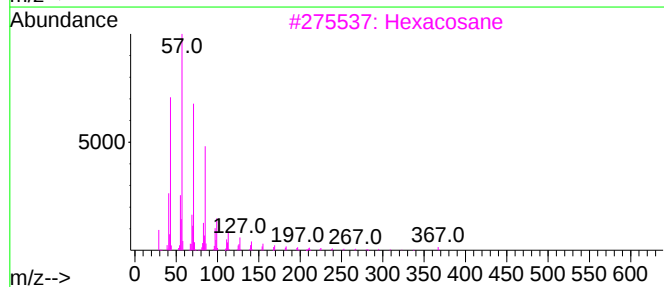
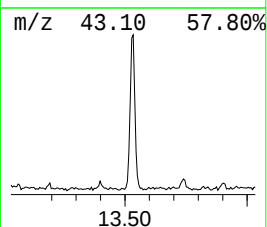
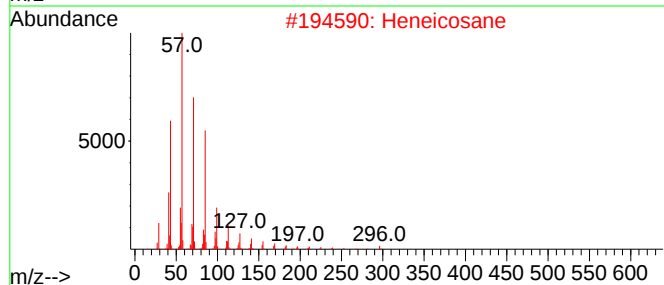
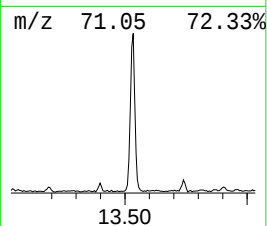
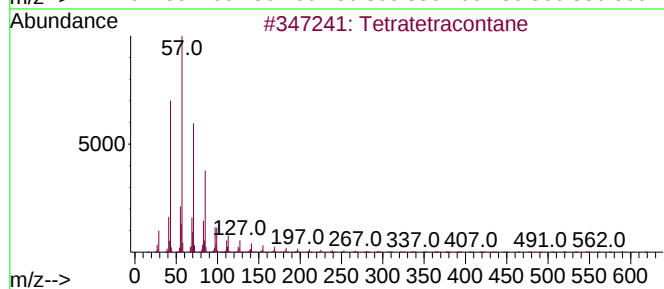
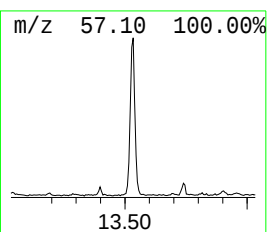
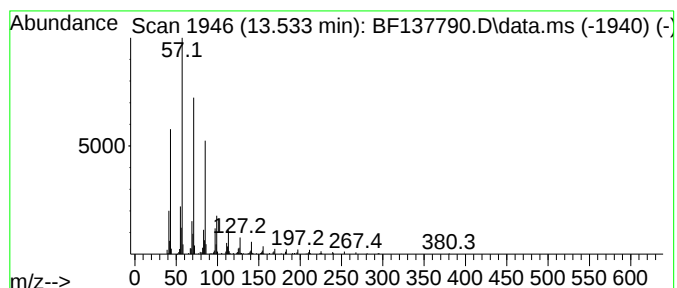
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.533	4.92 ng	336436	Chrysene-d12	14.251

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		Hexacosane	366	C26H54	000630-01-3	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptacosane	380	C27H56	000593-49-7	91



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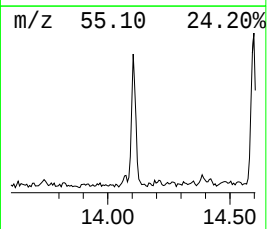
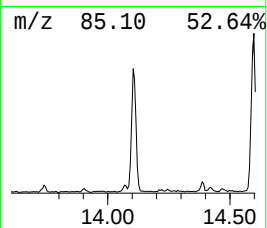
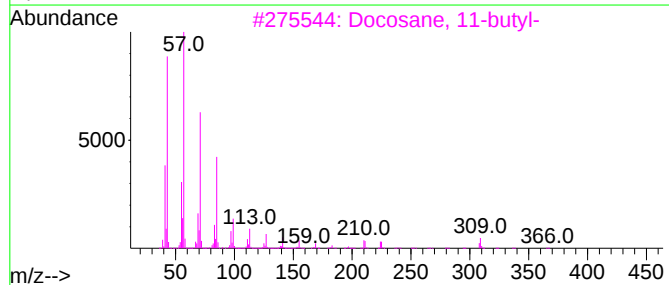
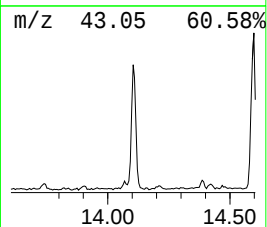
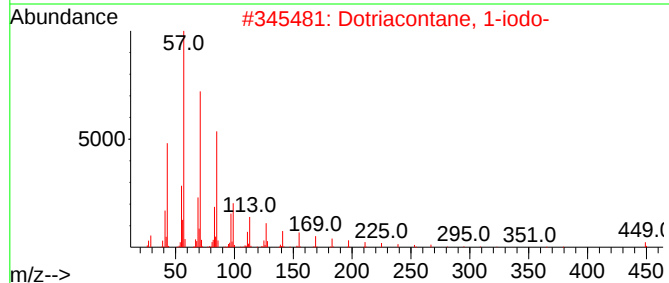
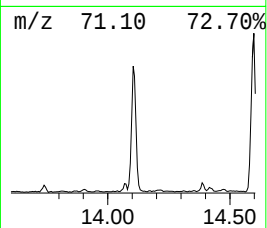
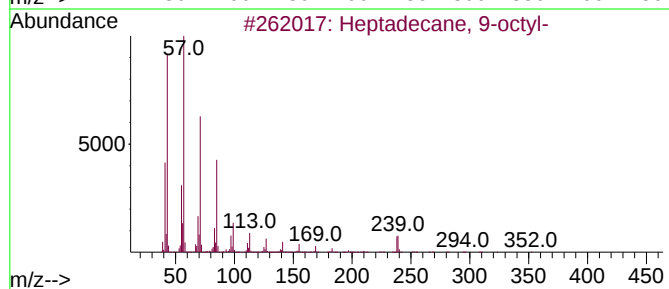
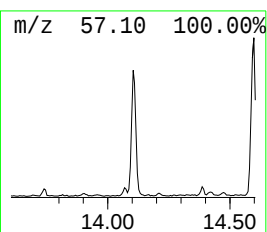
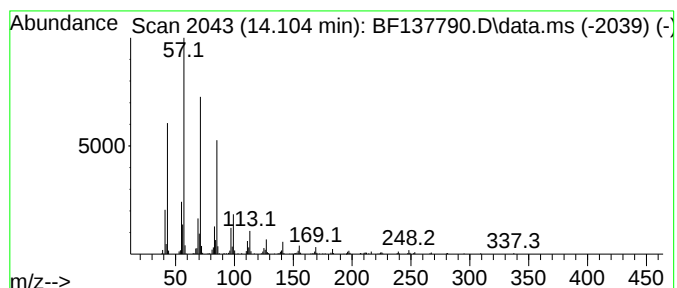
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EB-20240429

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.104	6.15 ng	420633	Chrysene-d12		14.251	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
2	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91
3	Docosane, 11-butyl-		366	C26H54	013475-76-8	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Docosane		310	C22H46	000629-97-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
Sample : P2306-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

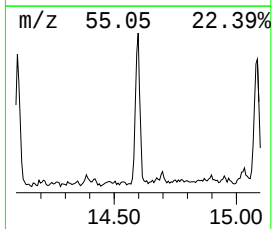
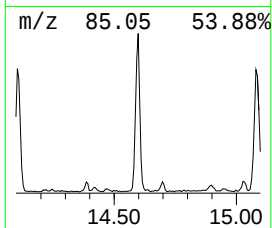
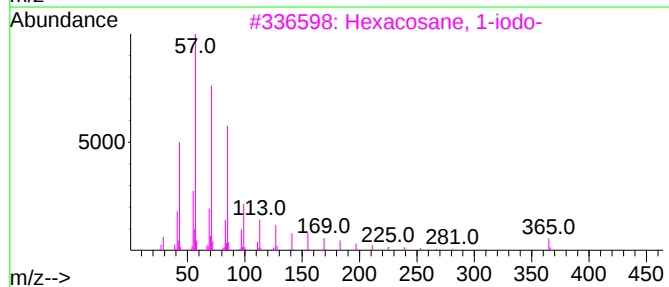
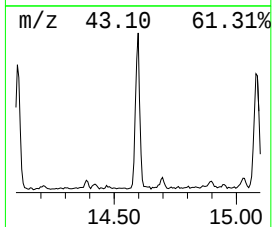
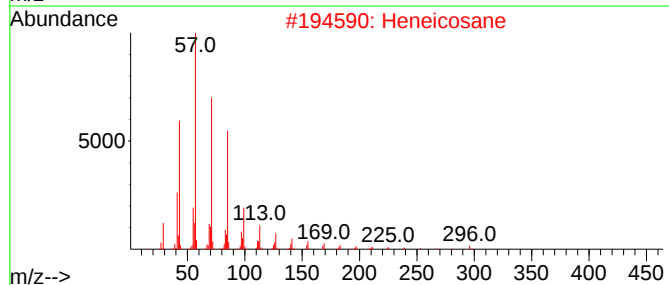
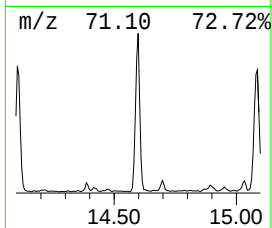
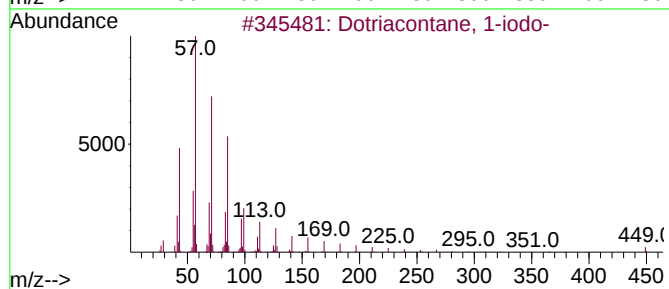
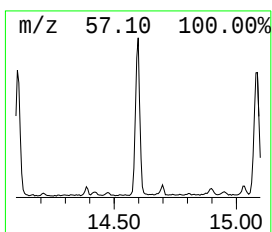
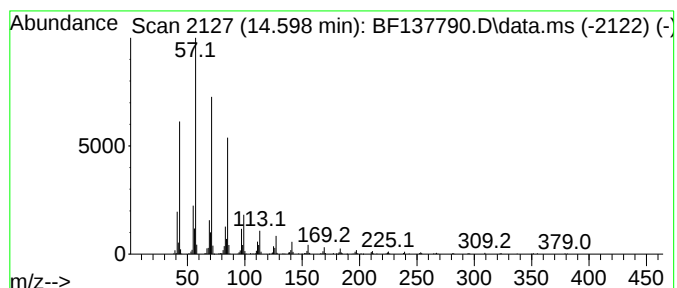
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.598	7.41 ng	506554	Chrysene-d12	14.251	
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	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
Sample : P2306-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-20240429

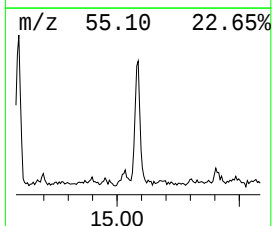
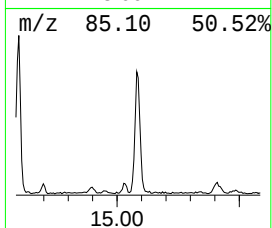
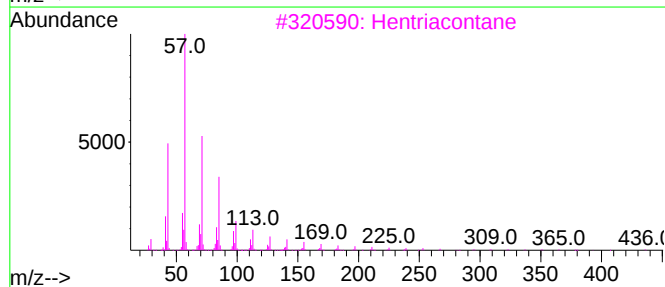
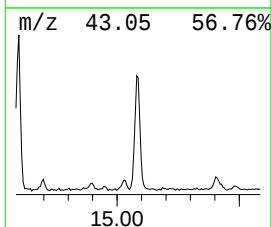
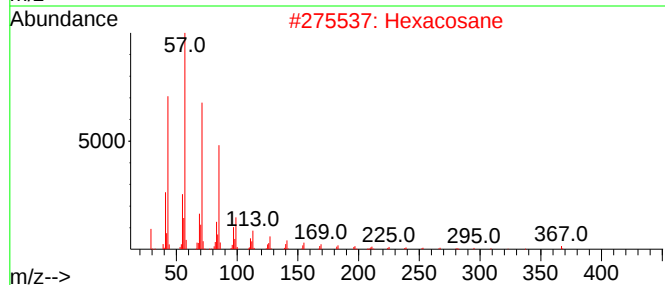
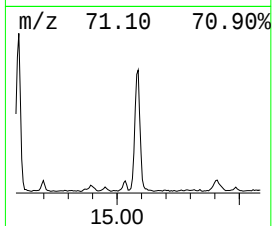
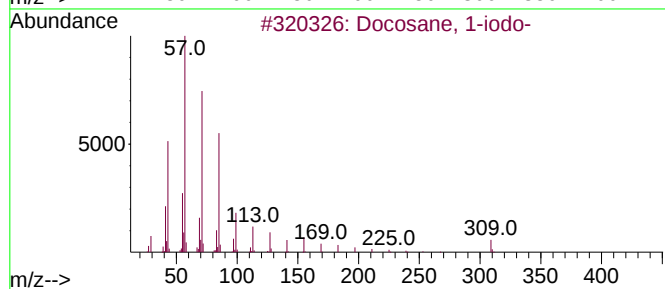
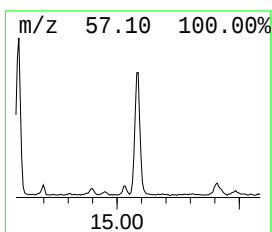
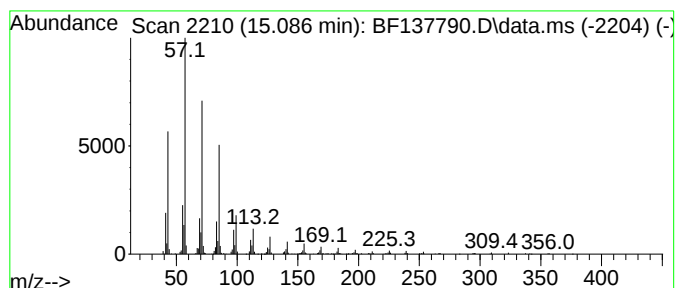
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	7.68 ng	488176	Perylene-d12	15.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
Sample : P2306-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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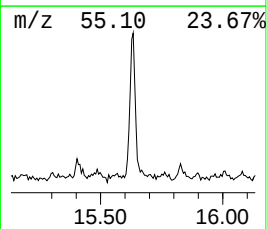
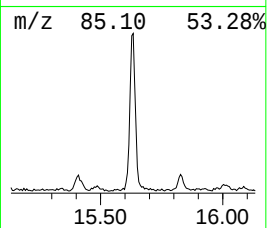
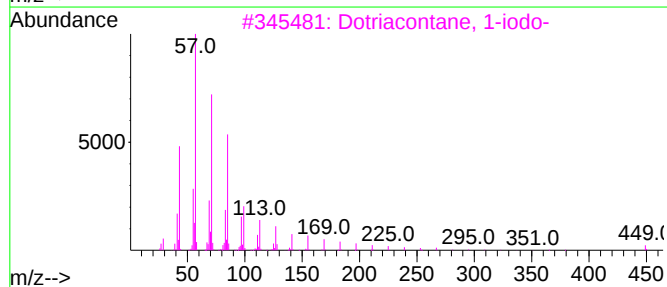
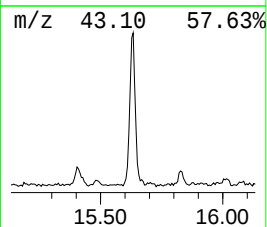
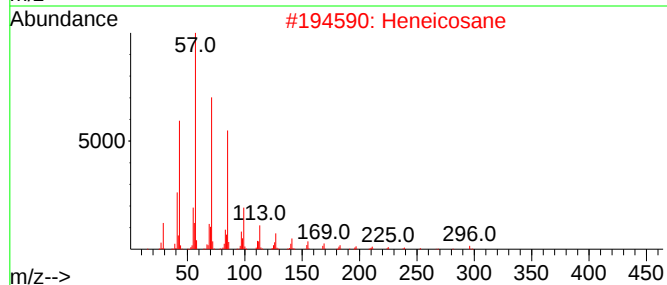
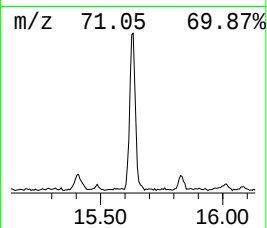
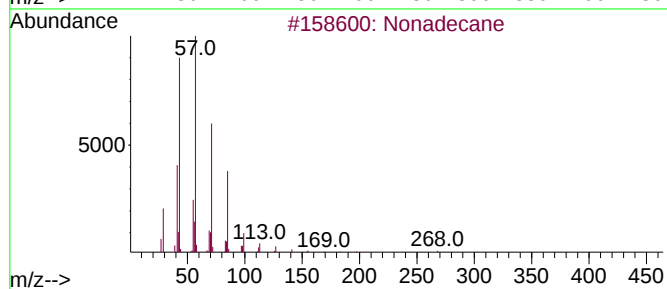
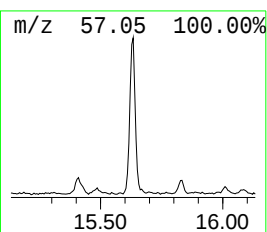
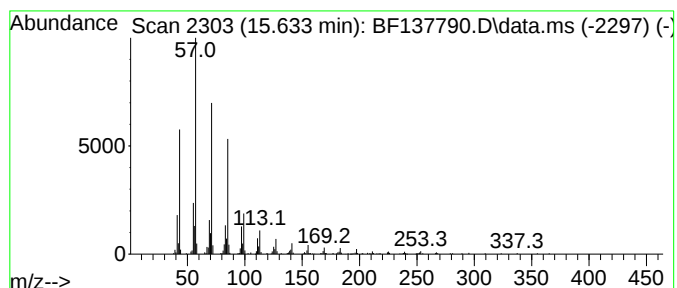
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.633	7.57 ng	481263	Perylene-d12	15.821

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	95
2		Heneicosane	296	C21H44	000629-94-7	91
3		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
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Instrument :
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ClientSampleId :
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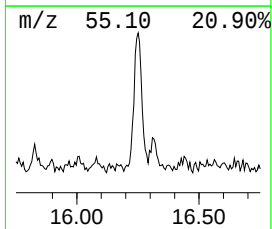
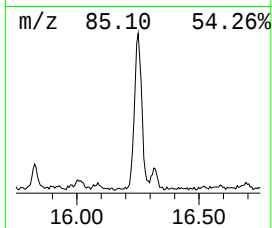
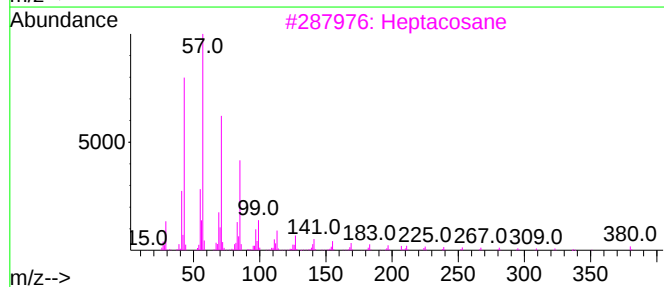
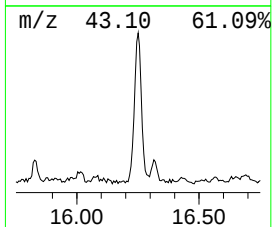
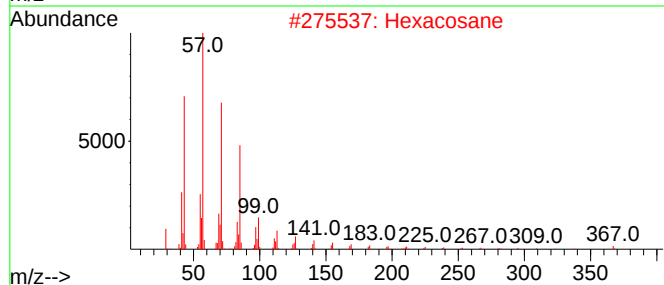
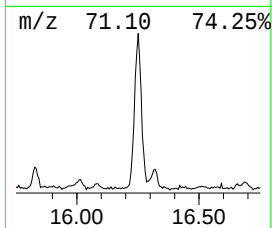
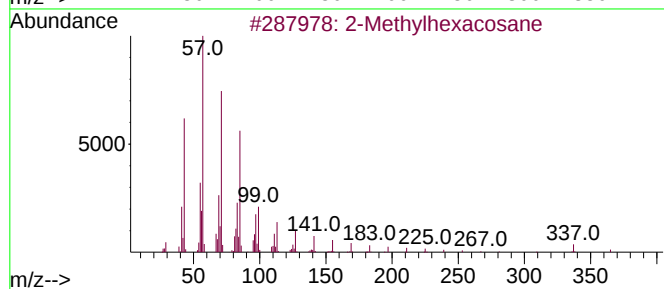
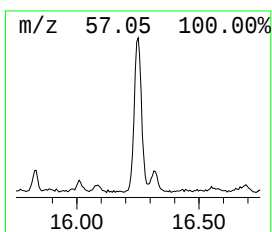
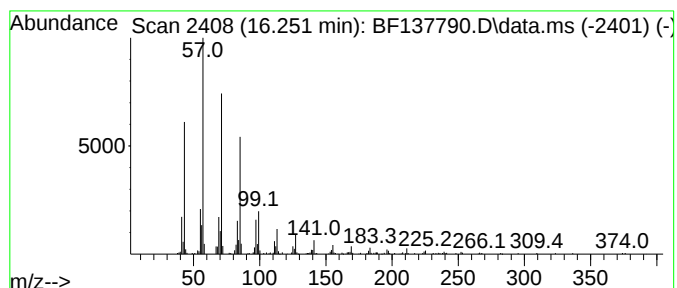
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-Methylhexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.251	6.15 ng	391313	Perylene-d12	15.821

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylhexacosane		380	C27H56	001561-02-0	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
Sample : P2306-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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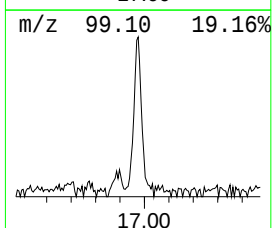
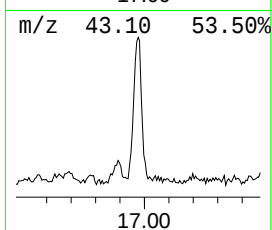
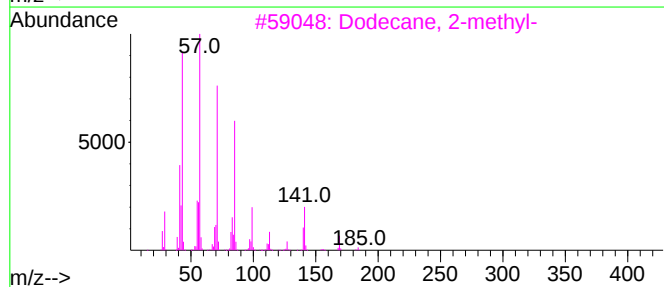
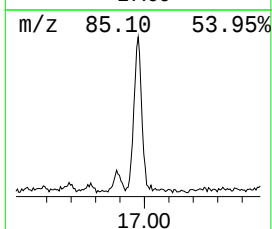
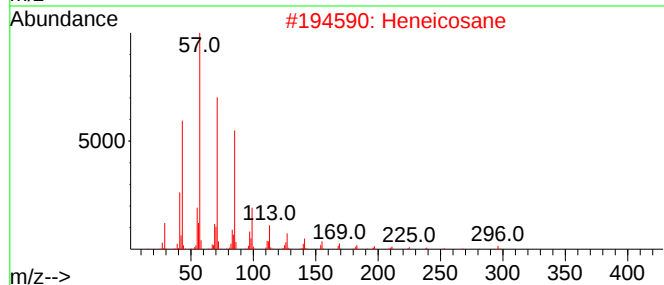
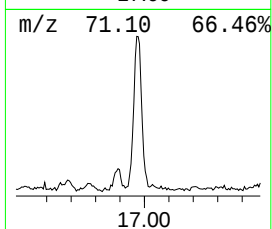
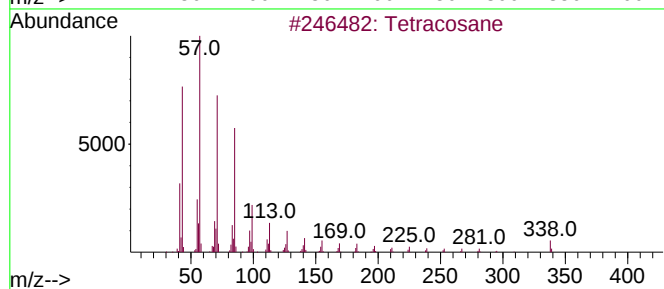
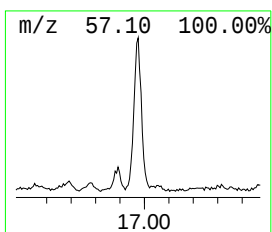
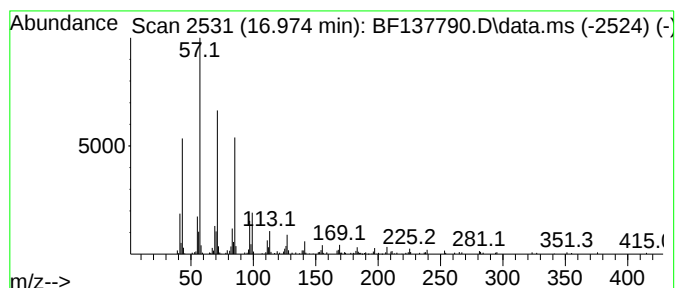
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.974	4.80 ng	305595	Perylene-d12	15.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4			Docosane	310	C22H46	000629-97-0	90
5			Triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
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Acq On : 01 May 2024 14:20
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Misc :
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ClientSampleId :
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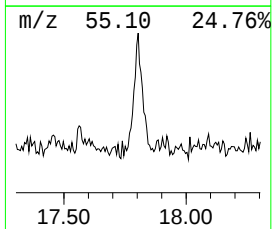
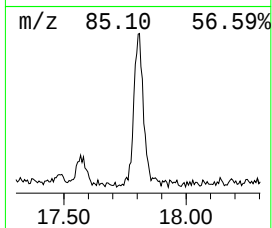
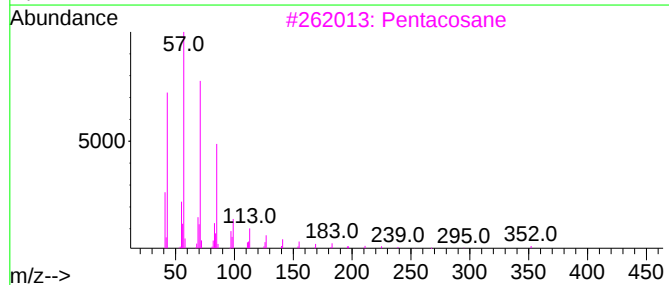
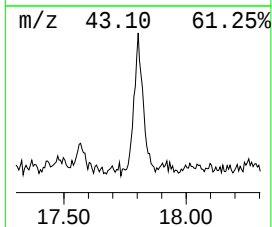
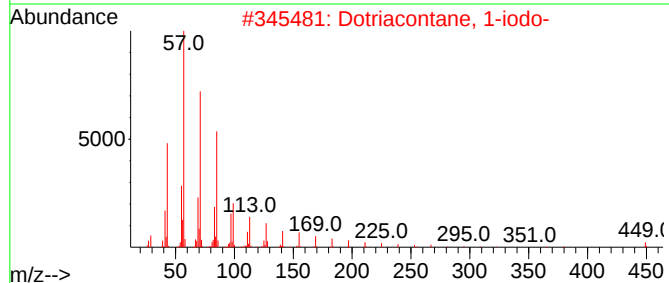
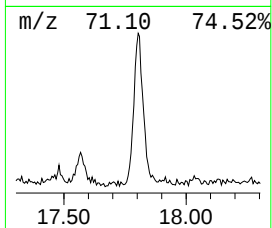
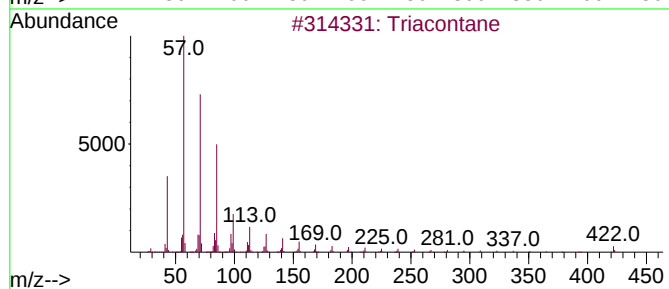
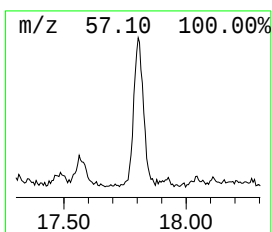
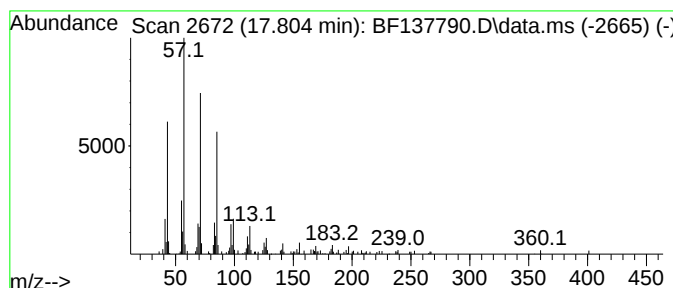
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.804	3.27 ng	208044	Perylene-d12	15.821

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
Sample : P2306-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EB-20240429

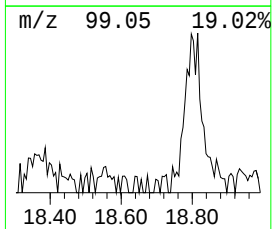
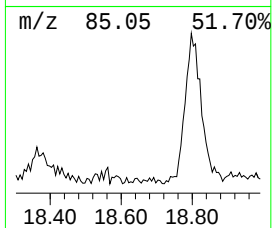
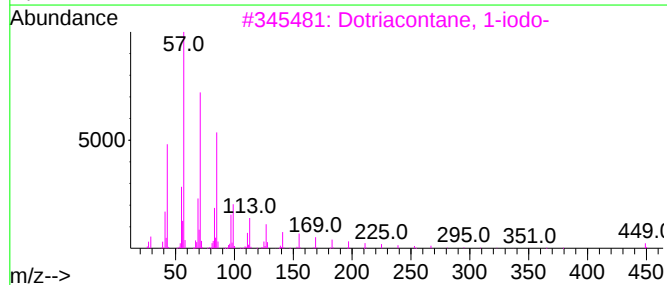
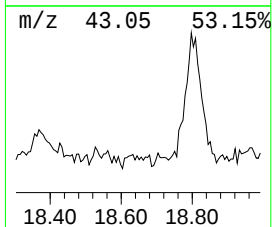
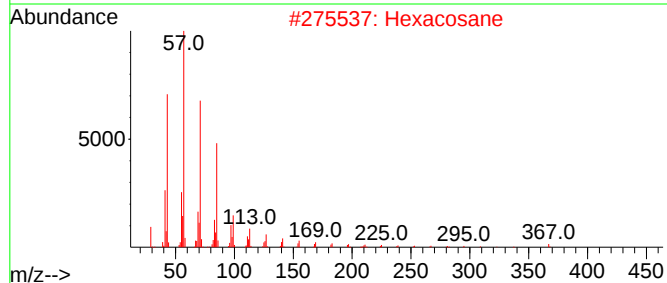
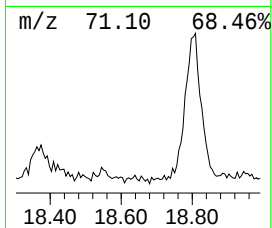
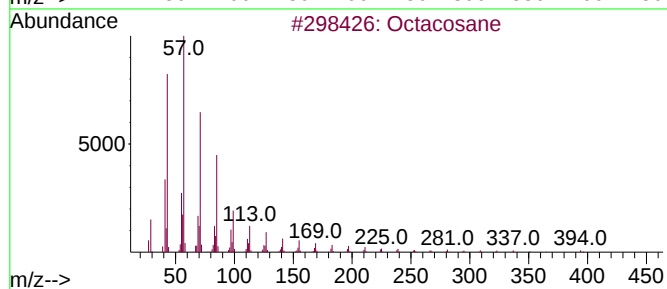
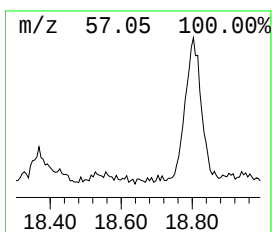
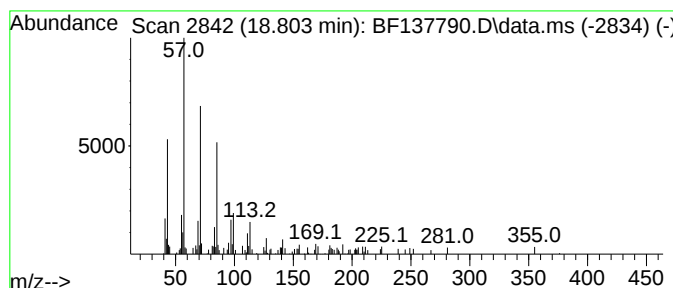
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.804	2.38 ng	151624	Perylene-d12	15.821

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
4		Pentacosane	352	C25H52	000629-99-2	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137790.D
Acq On : 01 May 2024 14:20
Operator : CG\JU
Sample : P2306-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-20240429

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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
Butane, 2-metho...	2.428	21.0	ng	1291240	1	7.057	1228360	20.0
n-Hexadecanoic ...	12.098	3.8	ng	381782	4	11.598	1999790	20.0
9-Octadecenoic ...	12.816	8.5	ng	846384	4	11.598	1999790	20.0
Octadecanoic acid	12.892	2.8	ng	281457	4	11.598	1999790	20.0
Tetratetracontane	13.533	4.9	ng	336436	5	14.251	1367930	20.0
Heptadecane, 9-...	14.104	6.2	ng	420633	5	14.251	1367930	20.0
Dotriacontane, ...	14.598	7.4	ng	506554	5	14.251	1367930	20.0
Docosane, 1-iodo-	15.086	7.7	ng	488176	6	15.821	1272050	20.0
Nonadecane	15.633	7.6	ng	481263	6	15.821	1272050	20.0
2-Methylhexacosane	16.251	6.2	ng	391313	6	15.821	1272050	20.0
Tetracosane	16.974	4.8	ng	305595	6	15.821	1272050	20.0
Triacontane	17.804	3.3	ng	208044	6	15.821	1272050	20.0
Octacosane	18.804	2.4	ng	151624	6	15.821	1272050	20.0