

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
 Data File : BF133571.D
 Acq On : 05 Jun 2023 18:05
 Operator : CG\JU
 Sample : 02986-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-13-0A

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	17	22	rBV	36301	49716	2.23%	0.253%
2	5.040	497	502	509	rBV	74407	87522	3.92%	0.445%
3	5.440	560	570	573	rBV	2378033	2231970	100.00%	11.344%
4	5.998	660	665	669	rVB	31464	31302	1.40%	0.159%
5	6.457	737	743	745	rBV	2217054	2206998	98.88%	11.217%
6	6.834	803	807	810	rBV	1015271	824243	36.93%	4.189%
7	6.887	813	816	819	rBV	33306	27781	1.24%	0.141%
8	7.010	834	837	840	rVB	95850	73669	3.30%	0.374%
9	7.392	898	902	905	rVB	1649641	1314878	58.91%	6.683%
10	8.116	1021	1025	1028	rBV	1333972	1039576	46.58%	5.284%
11	9.192	1204	1208	1211	rBV	2896713	2222064	99.56%	11.294%
12	9.869	1320	1323	1327	rBV	1225526	972069	43.55%	4.941%
13	10.580	1439	1444	1448	rBV	129540	117986	5.29%	0.600%
14	10.657	1453	1457	1460	rBV	1524276	1251049	56.05%	6.358%
15	11.357	1572	1576	1579	rBV	1125957	917482	41.11%	4.663%
16	11.886	1663	1666	1670	rBV	164023	153188	6.86%	0.779%
17	12.674	1797	1800	1806	rBV3	27335	35661	1.60%	0.181%
18	12.945	1842	1846	1850	rBV	2040864	1771149	79.35%	9.002%
19	13.180	1882	1886	1889	rBV	54910	54298	2.43%	0.276%
20	13.527	1942	1945	1947	rVB	39995	30850	1.38%	0.157%
21	13.880	1999	2005	2019	rBV2	276954	1039137	46.56%	5.281%
22	13.998	2022	2025	2029	rVB	757264	689370	30.89%	3.504%
23	14.174	2052	2055	2058	rBV	36172	36485	1.63%	0.185%
24	14.480	2104	2107	2109	rBV	80232	82282	3.69%	0.418%
25	14.516	2109	2113	2137	rVB3	404239	1405061	62.95%	7.141%
26	14.763	2153	2155	2157	rBV	50448	51646	2.31%	0.262%
27	15.121	2213	2216	2220	rVB	155193	167070	7.49%	0.849%
28	15.457	2269	2273	2276	rBV	399605	500278	22.41%	2.543%
29	15.486	2276	2278	2288	rVB	132647	191258	8.57%	0.972%
30	15.939	2352	2355	2360	rBV2	73869	99203	4.44%	0.504%

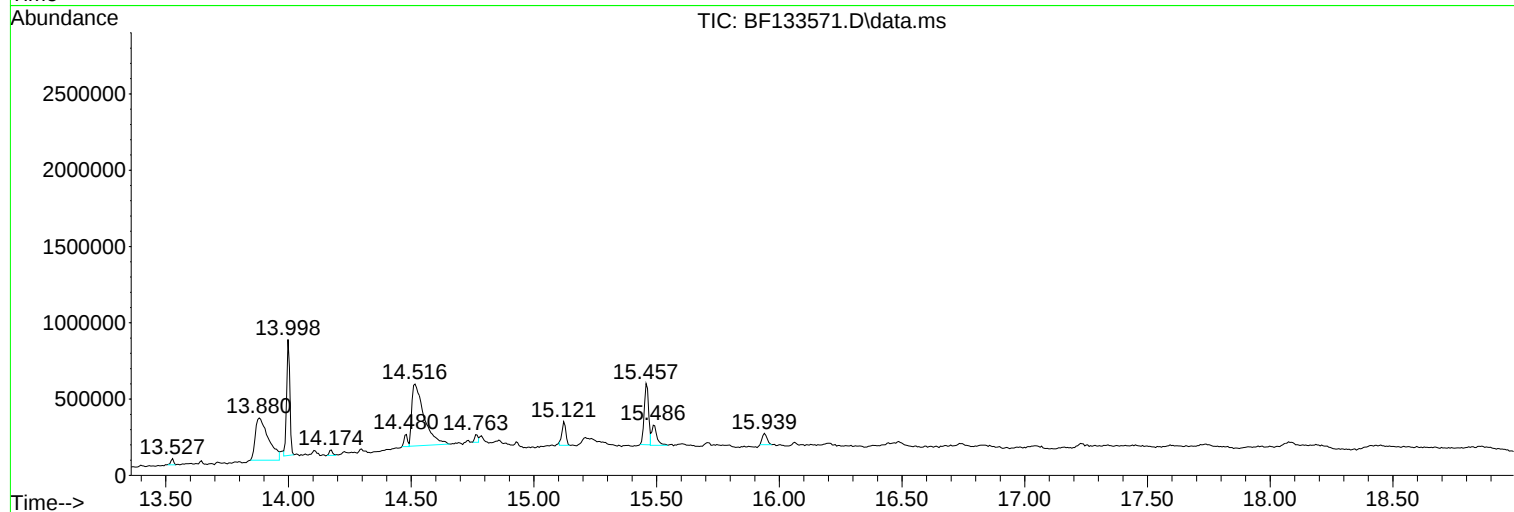
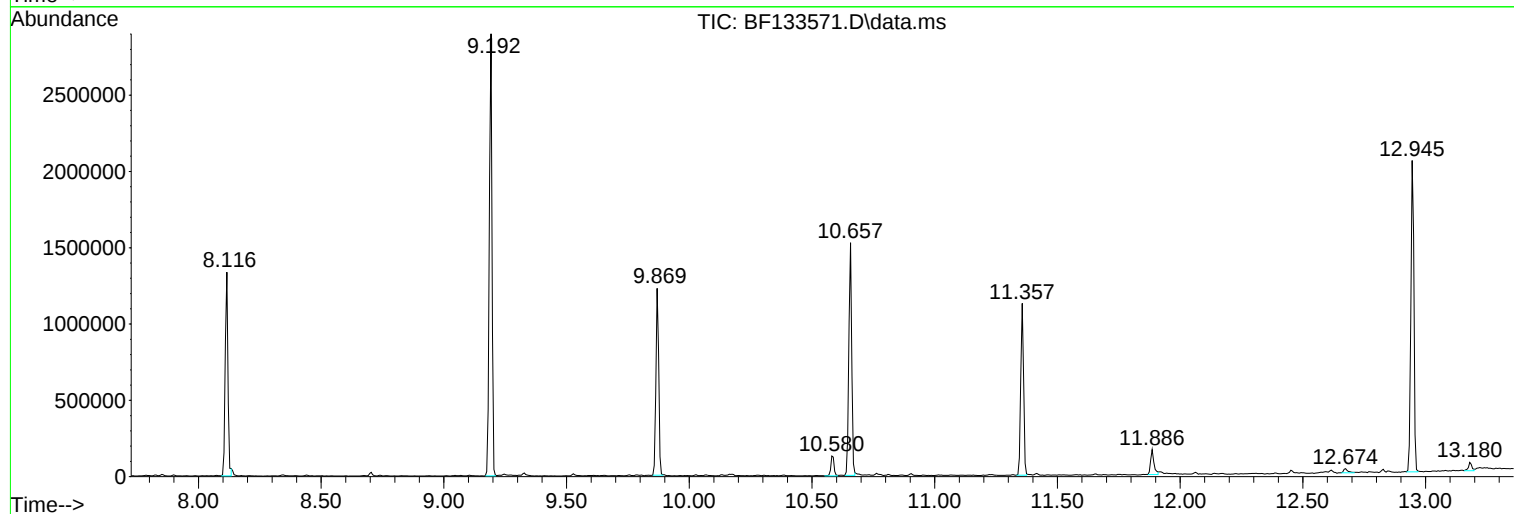
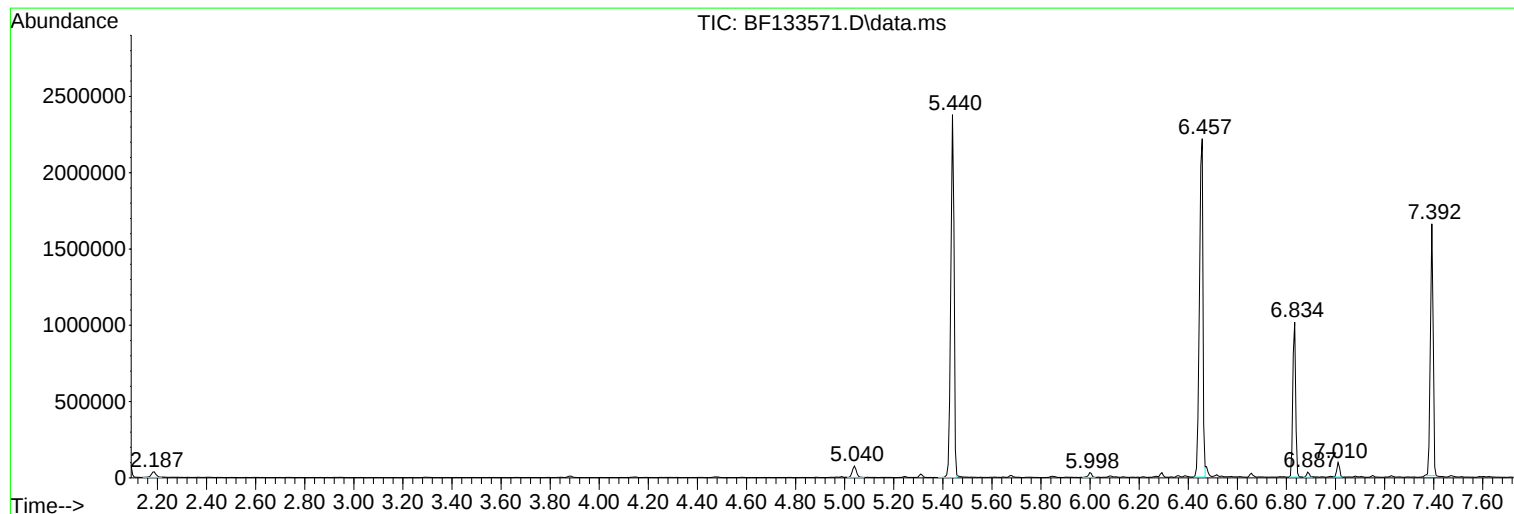
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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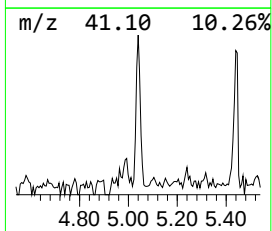
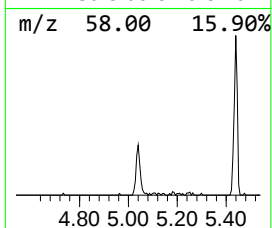
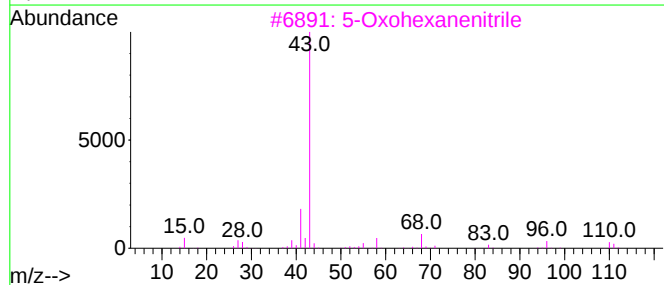
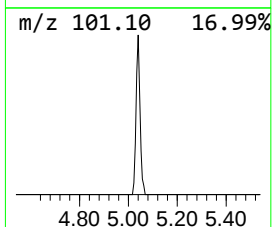
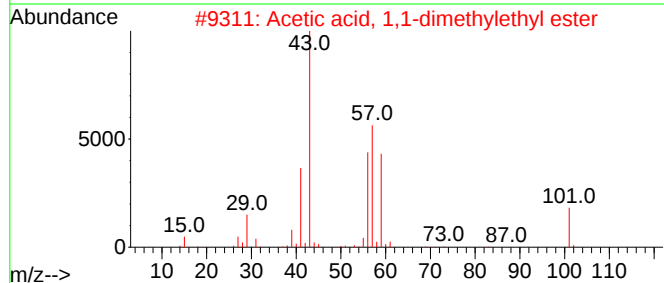
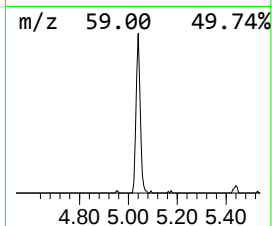
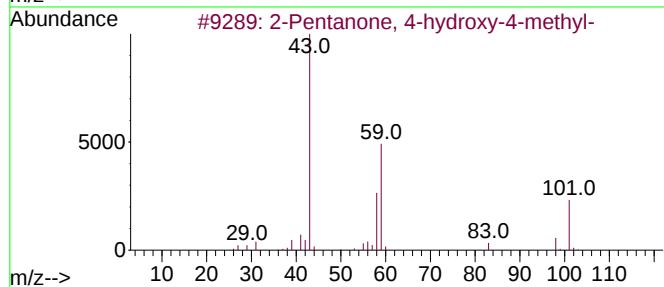
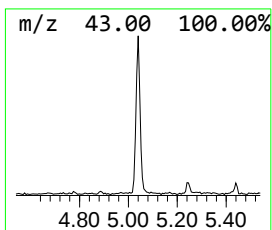
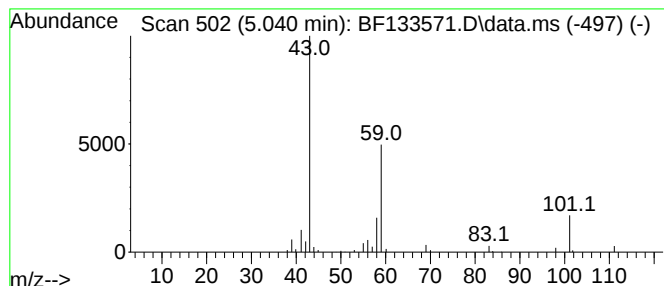
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.12 ng	87522	1,4-Dichlorobenzene-d4	6.834

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	39		
3	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	22		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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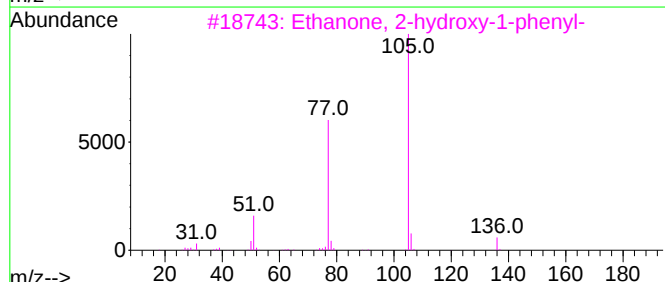
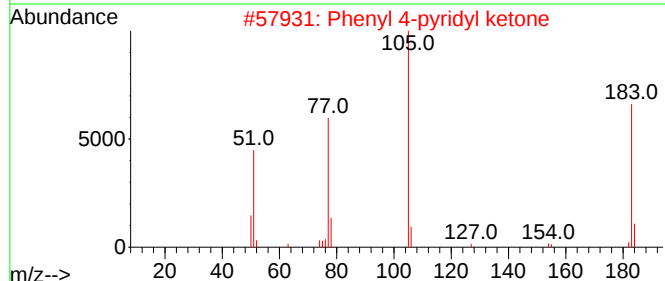
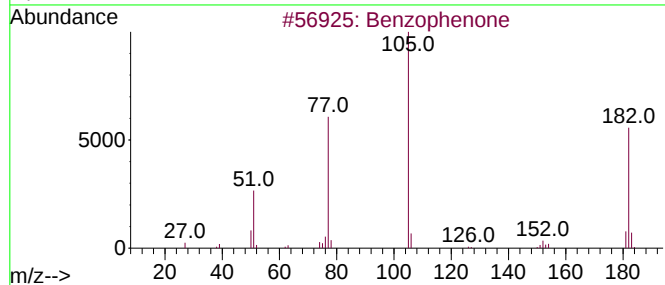
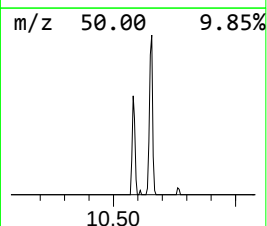
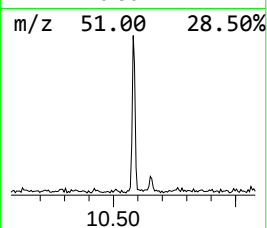
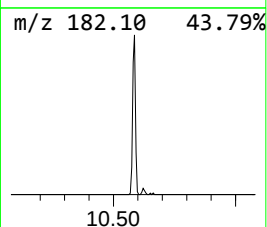
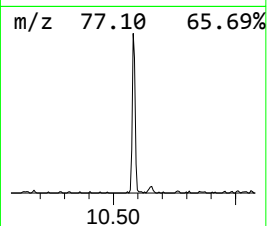
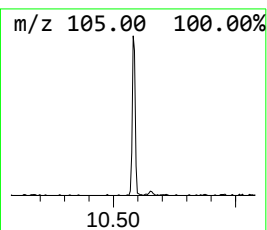
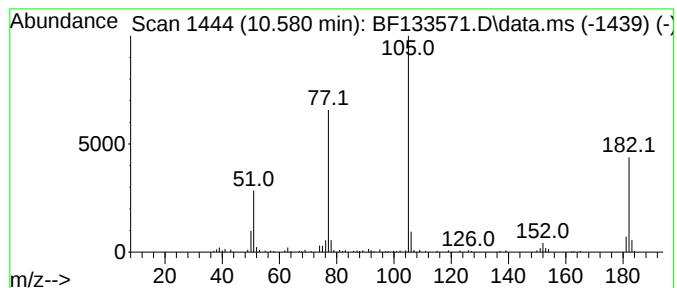
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.581	2.43 ng	117986	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	50
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50



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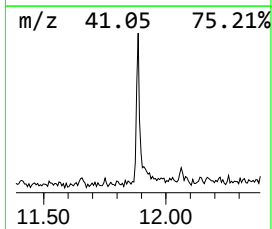
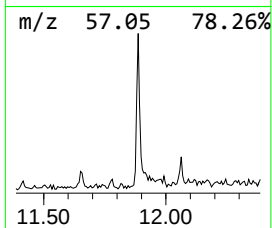
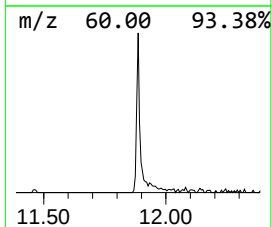
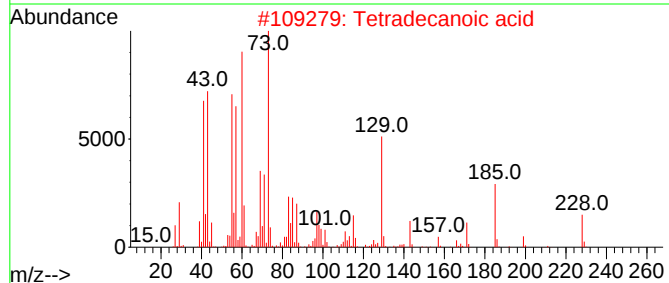
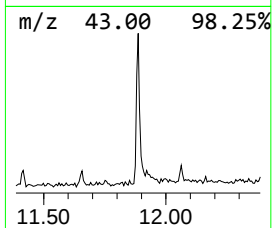
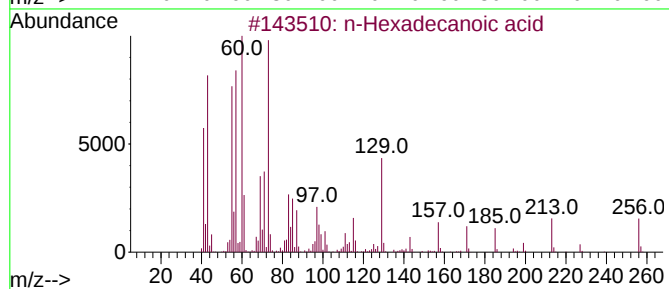
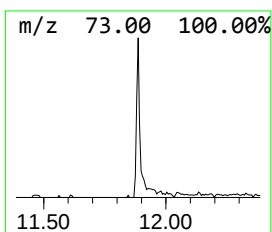
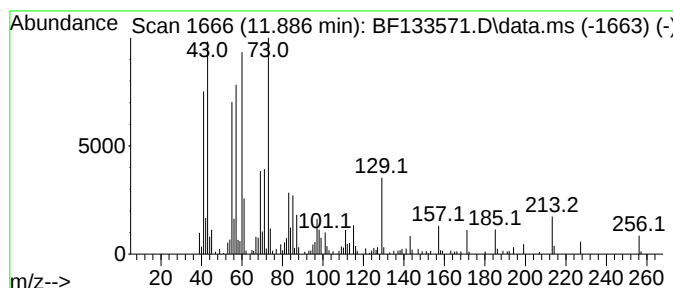
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BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.886	3.34 ng	153188	Phenanthrene-d10	11.357	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	81



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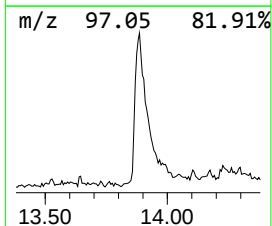
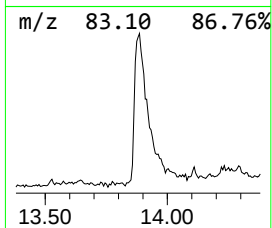
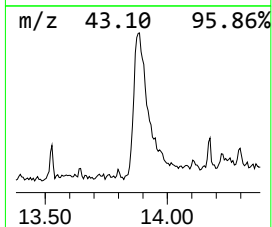
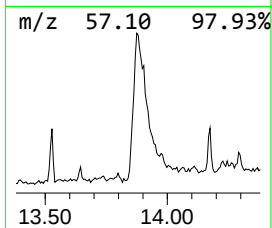
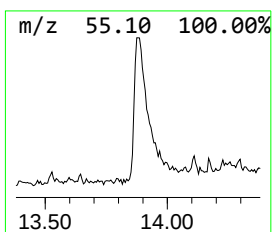
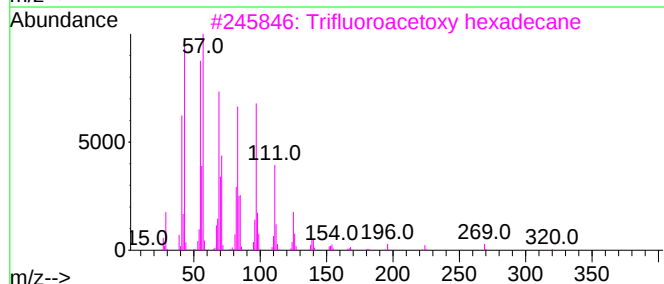
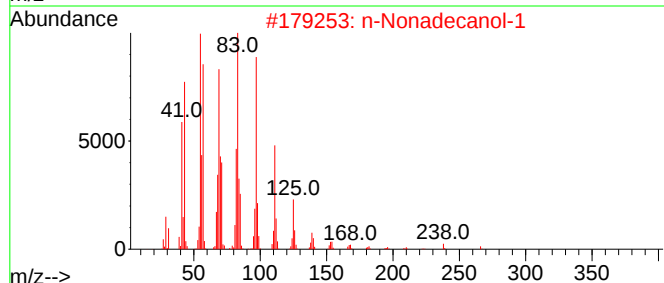
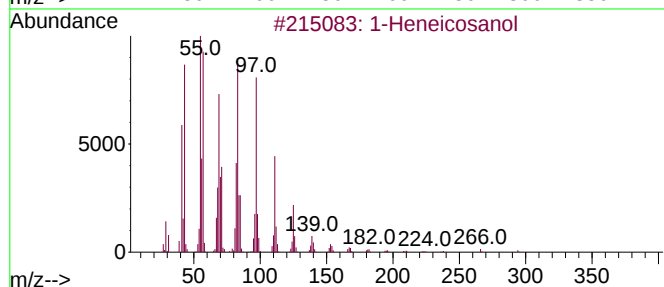
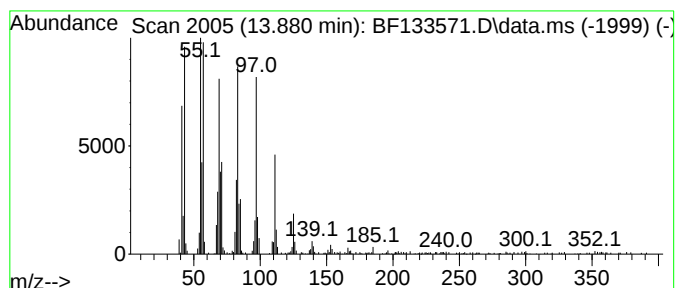
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.880	30.15 ng	1039140	Chrysene-d12	13.998	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	10-Heneicosene (c,t)	294	C21H42	095008-11-0	93



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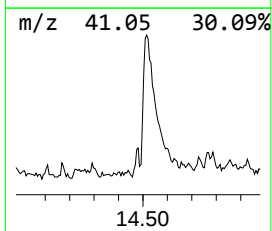
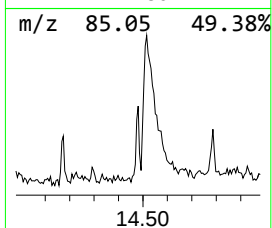
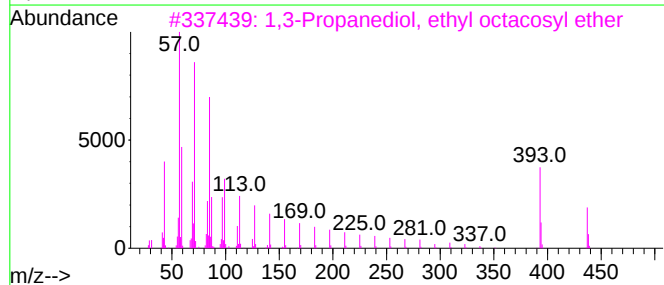
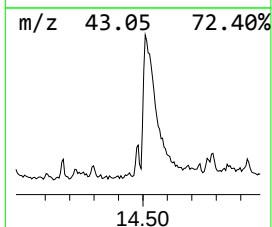
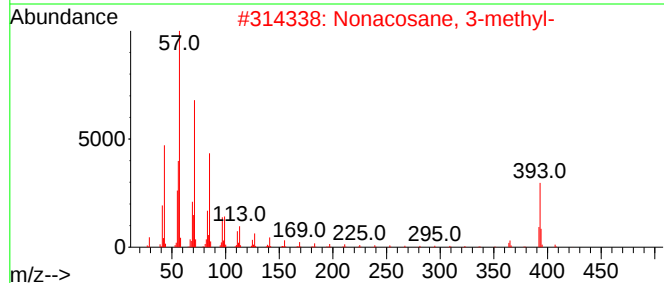
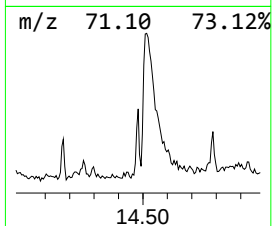
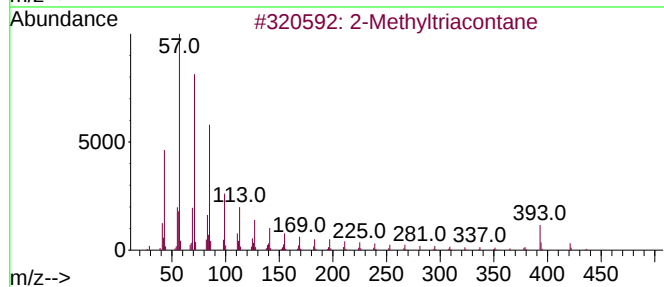
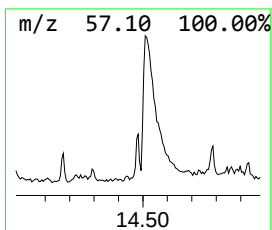
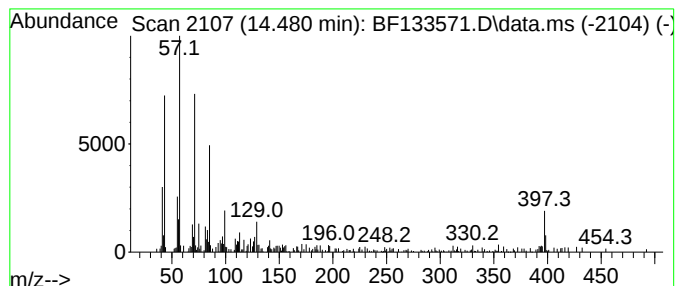
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Methyltriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	2.39 ng	82282	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyltriacontane	437	C31H64	001560-72-1	64
2			Nonacosane, 3-methyl-	422	C30H62	014167-67-0	50
3			1,3-Propanediol, ethyl octacosyl...	497	C33H68O2	1000406-35-9	50
4			Isopropyl octacosyl ether	452	C31H64O	1010406-34-7	25
5			1-Heptadecanamine	255	C17H37N	004200-95-7	9



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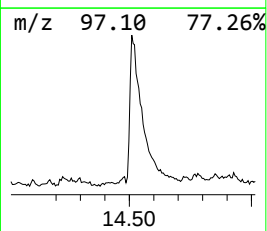
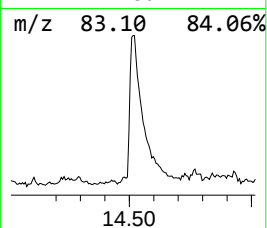
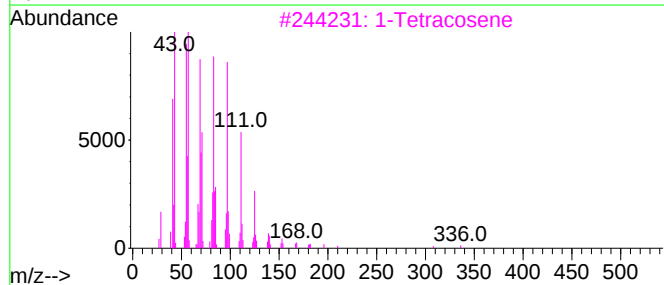
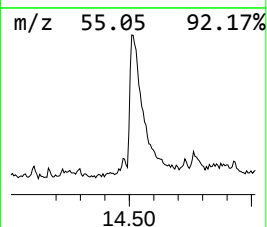
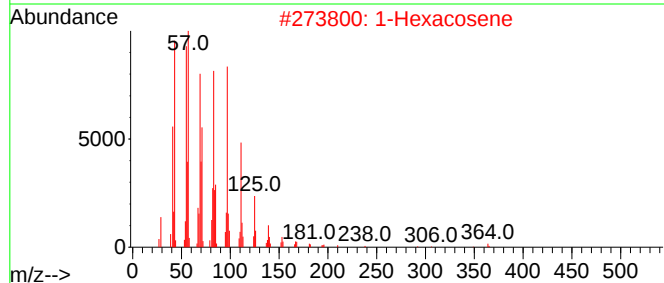
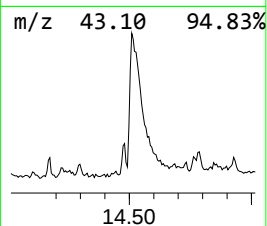
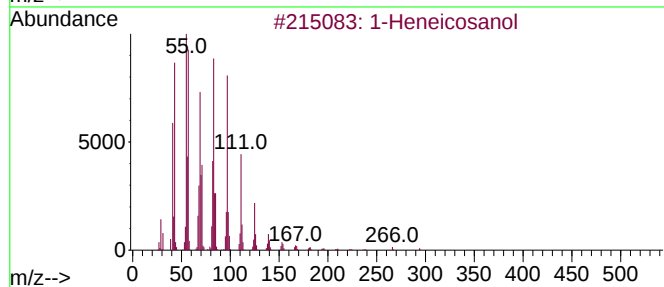
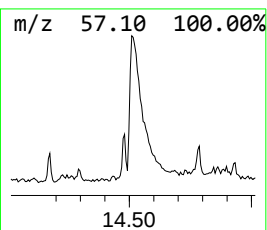
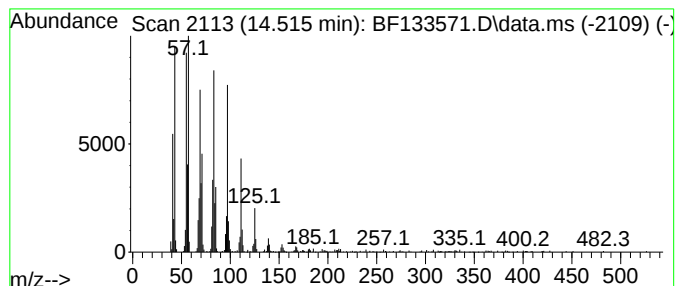
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexacosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	40.76 ng	1405060	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			1-Tetracosene	336	C24H48	010192-32-2	94
4			1-Docosene	308	C22H44	001599-67-3	93
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133571.D
Acq On : 05 Jun 2023 18:05
Operator : CG\JU
Sample : 02986-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13-0A

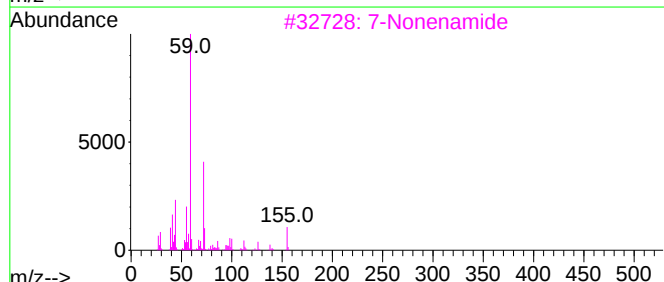
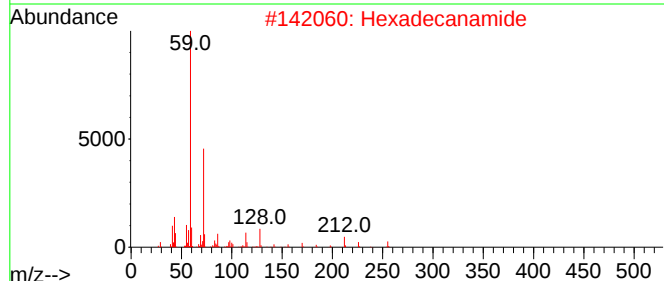
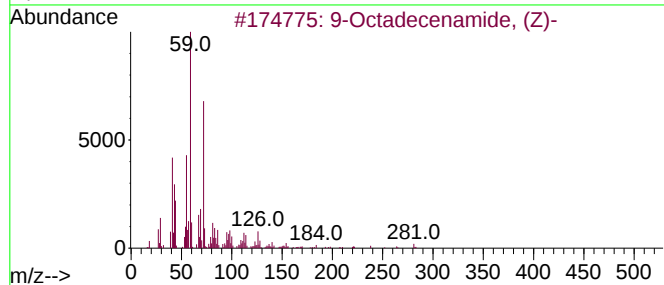
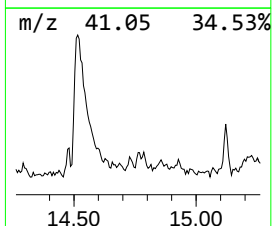
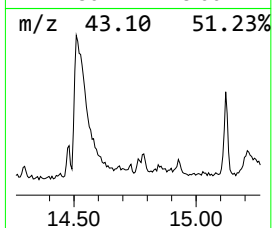
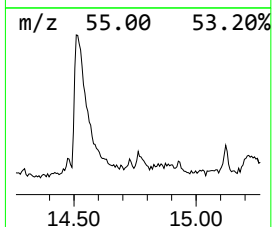
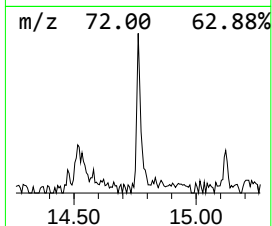
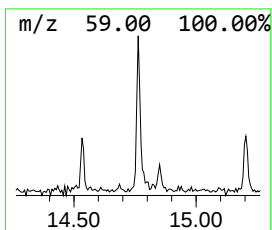
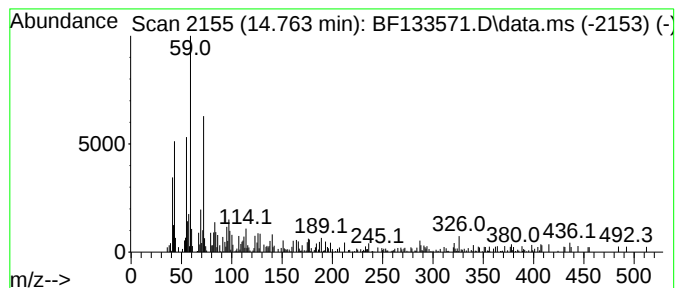
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	2.06 ng	51646	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2		Hexadecanamide	255	C16H33NO	000629-54-9	64
3		7-Nonenamide	155	C9H17NO	090949-53-4	64
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	53
5		Tetradecanamide	227	C14H29NO	000638-58-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133571.D
Acq On : 05 Jun 2023 18:05
Operator : CG\JU
Sample : 02986-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13-0A

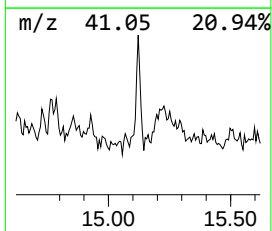
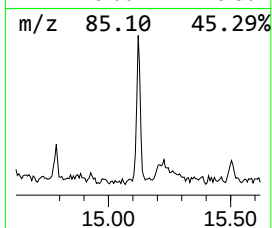
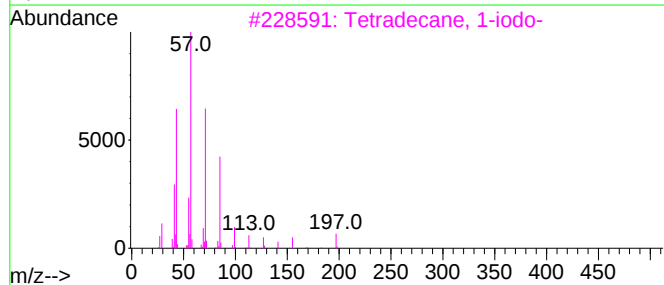
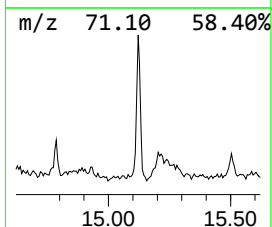
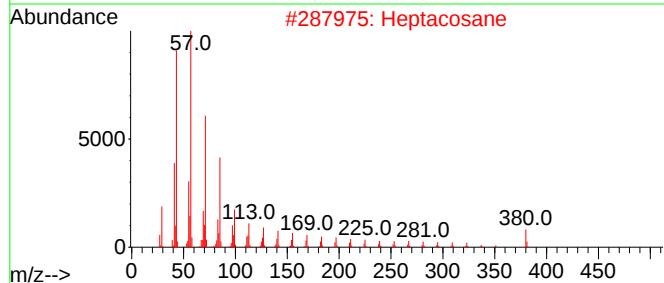
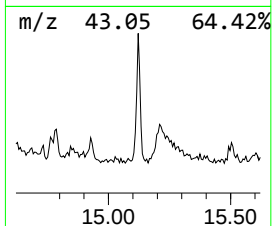
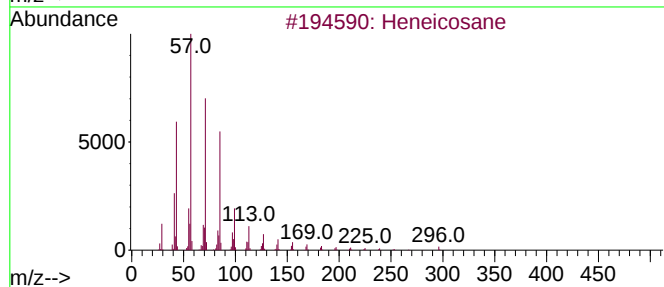
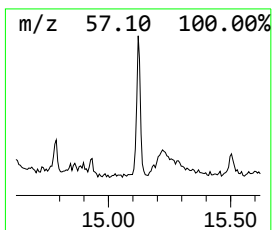
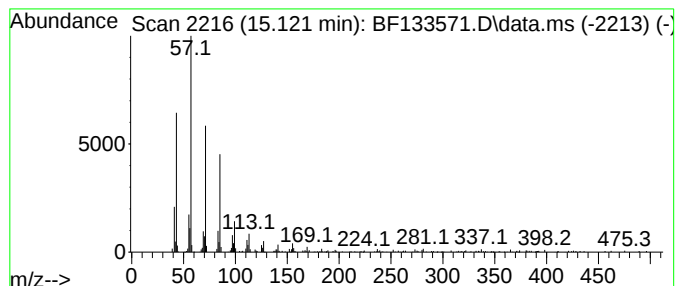
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	6.68 ng	167070	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Heptacosane	380	C27H56	000593-49-7	83
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
4			Tetracosane	338	C24H50	000646-31-1	83
5			Eicosane	282	C20H42	000112-95-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133571.D
Acq On : 05 Jun 2023 18:05
Operator : CG\JU
Sample : 02986-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13-0A

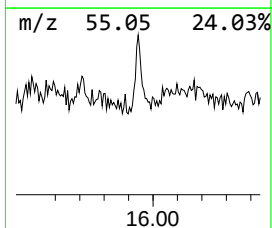
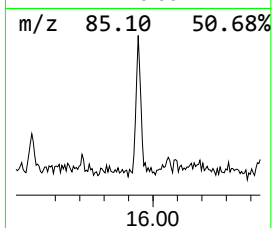
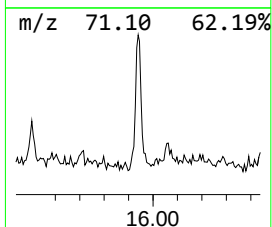
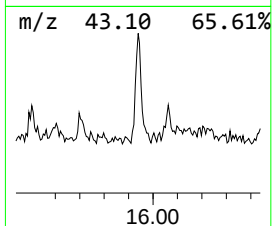
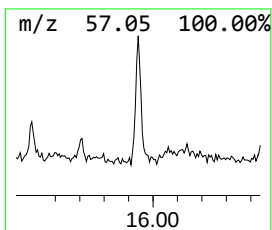
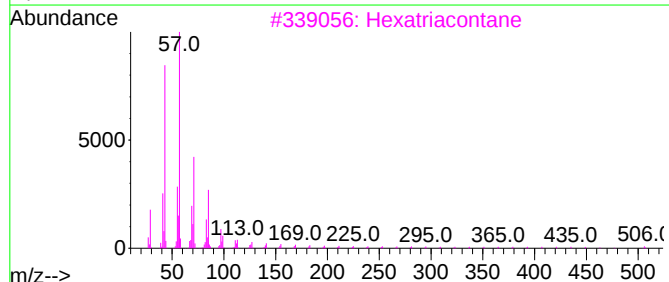
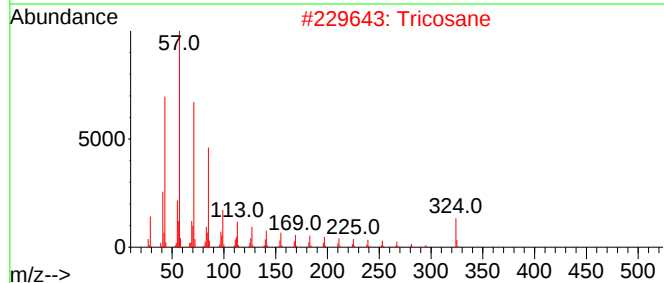
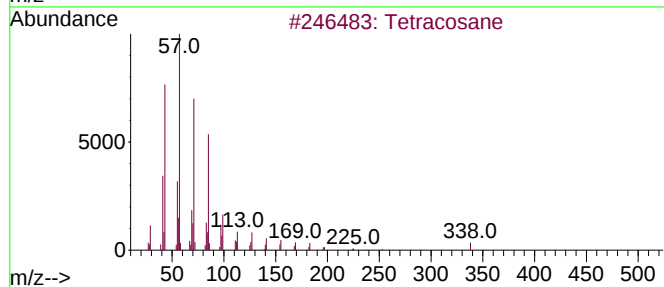
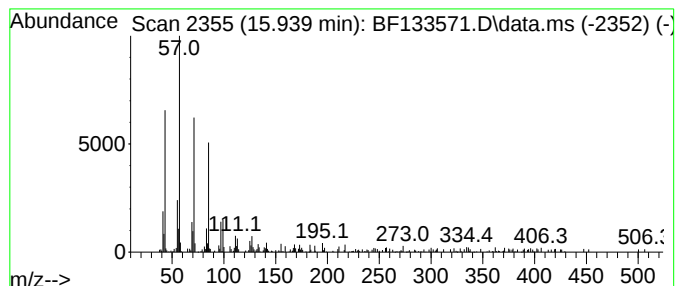
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	3.97 ng	99203	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Tricosane	324	C23H48	000638-67-5	81
3			Hexatriacontane	507	C36H74	000630-06-8	81
4			Tricosane, 2-methyl-	338	C24H50	001928-30-9	72
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133571.D
Acq On : 05 Jun 2023 18:05
Operator : CG\JU
Sample : 02986-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-13-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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-...	5.040	2.1	ng	87522	1	6.834	824243	20.0
Benzophenone	10.581	2.4	ng	117986	3	9.869	972069	20.0
n-Hexadecanoic ...	11.886	3.3	ng	153188	4	11.357	917482	20.0
1-Heneicosanol	13.880	30.1	ng	1039140	5	13.998	689370	20.0
2-Methyltriacon...	14.480	2.4	ng	82282	5	13.998	689370	20.0
1-Hexacosene	14.515	40.8	ng	1405060	5	13.998	689370	20.0
9-Octadecenamid...	14.763	2.1	ng	51646	6	15.457	500278	20.0
Heneicosane	15.121	6.7	ng	167070	6	15.457	500278	20.0
Tetracosane	15.939	4.0	ng	99203	6	15.457	500278	20.0