

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
 Data File : BF135257.D
 Acq On : 14 Sep 2023 16:49
 Operator : CG\JU
 Sample : 04338-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP4

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135257.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	14	18	28	rVB	40311	58495	1.25%	0.188%
2	5.028	496	500	509	rVB	89422	152169	3.25%	0.490%
3	5.404	559	564	567	rBV	3390956	4073080	86.94%	13.103%
4	6.410	729	735	738	rBV	3298877	4163504	88.87%	13.394%
5	6.757	791	794	798	rBV	850152	767981	16.39%	2.471%
6	7.328	885	891	894	rBV	2577432	2989658	63.82%	9.618%
7	8.039	1005	1012	1015	rBV	1198994	1102576	23.54%	3.547%
8	9.122	1189	1196	1199	rBV	4401056	4684751	100.00%	15.071%
9	9.798	1305	1311	1314	rBV	1241878	1168750	24.95%	3.760%
10	10.004	1341	1346	1352	rBV	37575	48538	1.04%	0.156%
11	10.592	1440	1446	1449	rBV	2742006	2885115	61.59%	9.281%
12	11.286	1560	1564	1567	rBV	1359408	1192120	25.45%	3.835%
13	11.827	1648	1656	1667	rBV	608068	707056	15.09%	2.275%
14	12.098	1693	1702	1704	rBV2	81308	182439	3.89%	0.587%
15	12.116	1704	1705	1716	rVB	106908	185796	3.97%	0.598%
16	12.510	1768	1772	1775	rBV	37062	56156	1.20%	0.181%
17	12.616	1785	1790	1799	rBV	190415	223885	4.78%	0.720%
18	12.892	1832	1837	1840	rBV	3797097	3802936	81.18%	12.234%
19	13.068	1861	1867	1874	rBV4	25488	60157	1.28%	0.194%
20	13.468	1929	1935	1938	rBV2	64267	63341	1.35%	0.204%
21	13.798	1987	1991	1994	rBV	108195	97372	2.08%	0.313%
22	13.845	1994	1999	2012	rVV3	105993	283054	6.04%	0.911%
23	13.945	2012	2016	2020	rBV	847154	731146	15.61%	2.352%
24	14.115	2042	2045	2049	rBV	108863	100899	2.15%	0.325%
25	14.427	2094	2098	2100	rBV	100676	93804	2.00%	0.302%
26	14.710	2142	2146	2154	rBV2	347930	447831	9.56%	1.441%
27	15.068	2204	2207	2213	rVB	47908	59840	1.28%	0.193%
28	15.409	2260	2265	2269	rBV	585593	702598	15.00%	2.260%

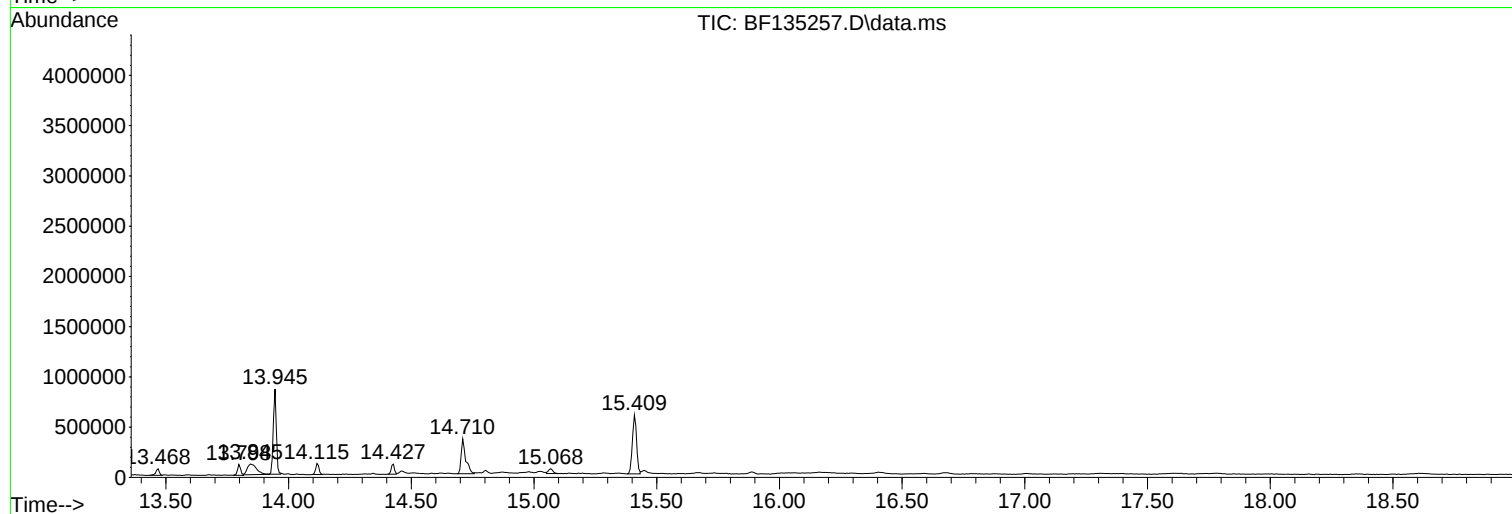
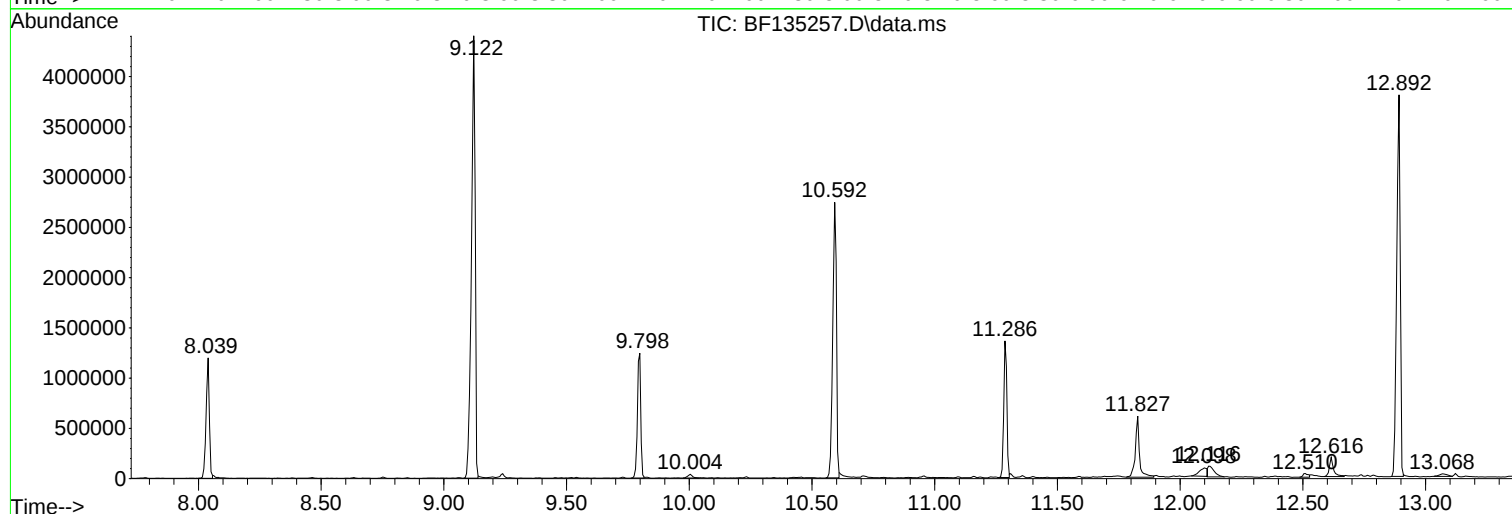
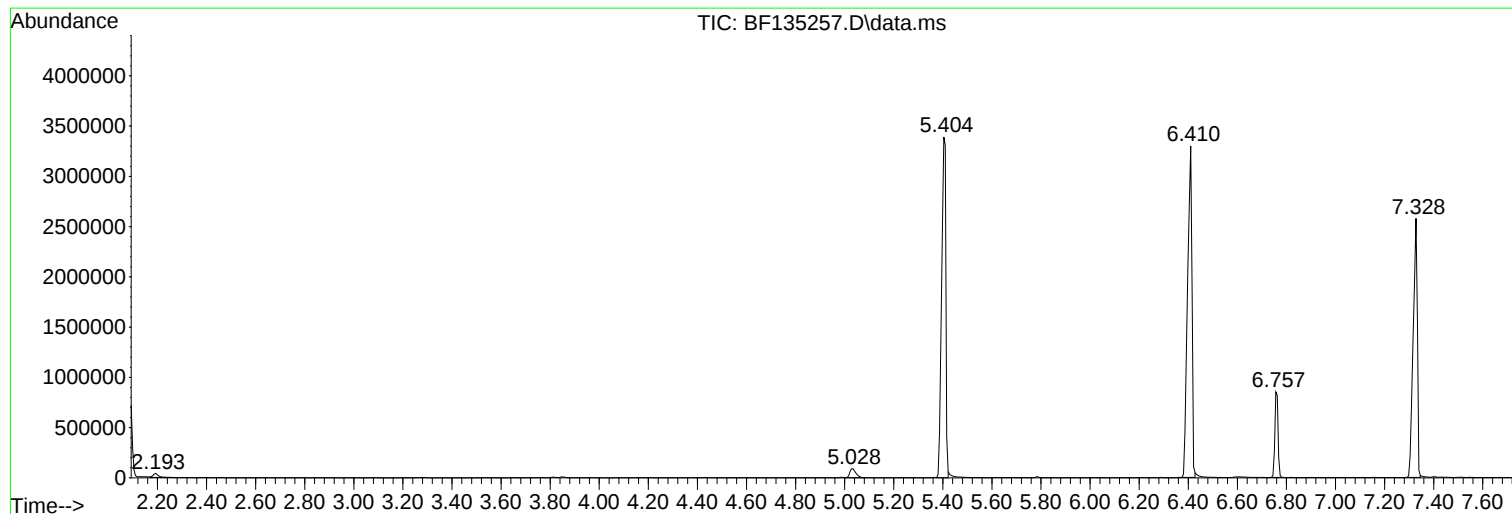
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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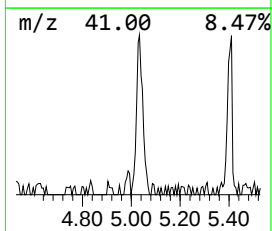
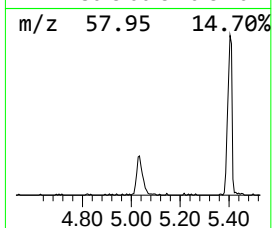
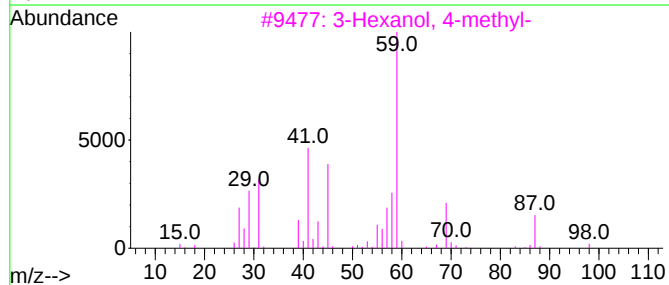
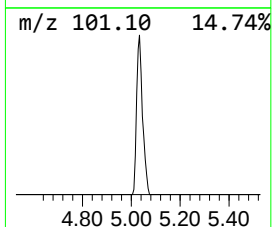
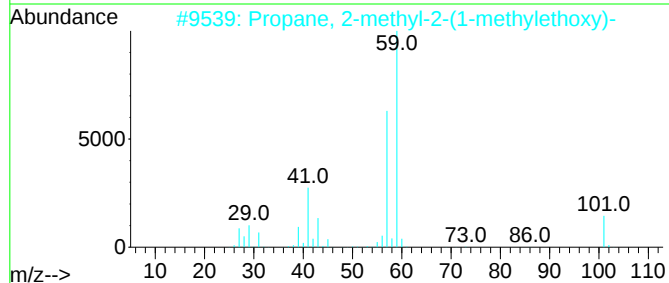
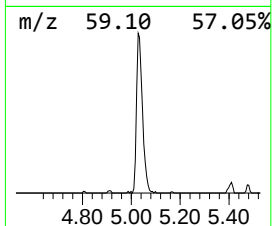
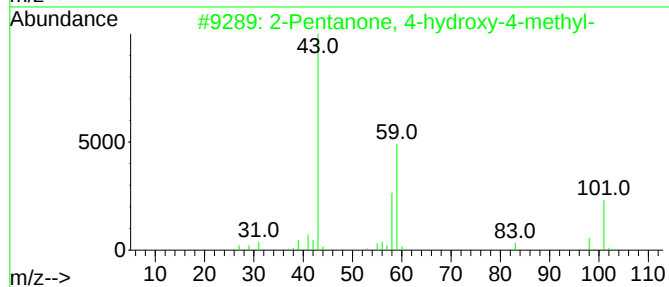
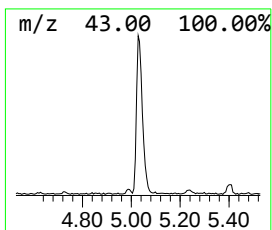
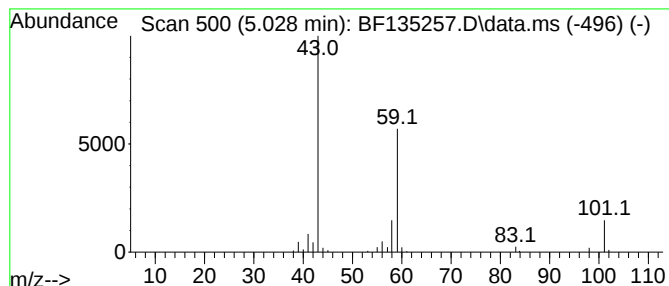
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	3.96 ng	152169	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	3-Octanol	130	C8H18O	000589-98-0	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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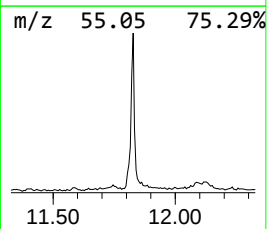
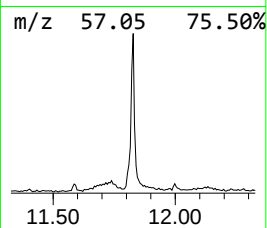
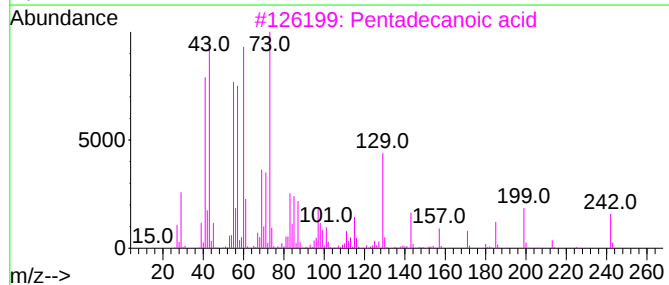
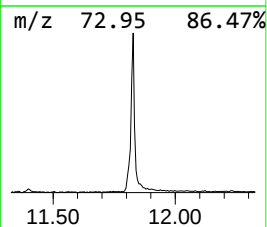
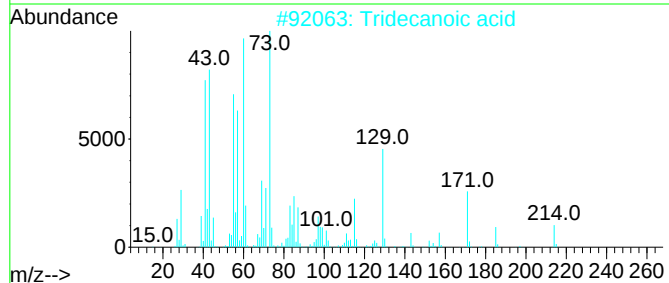
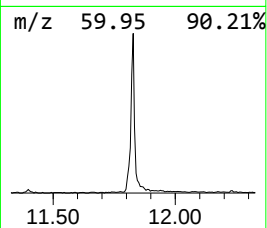
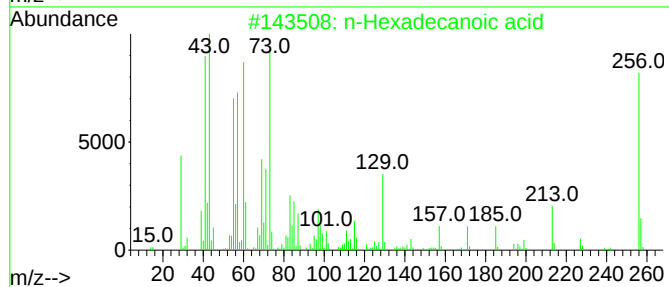
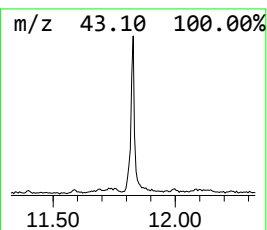
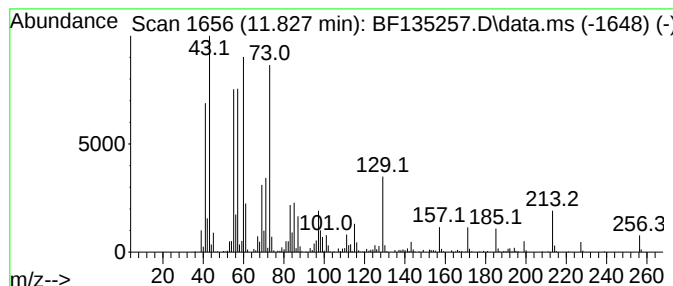
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	11.86 ng	707056	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	49



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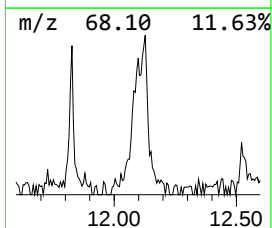
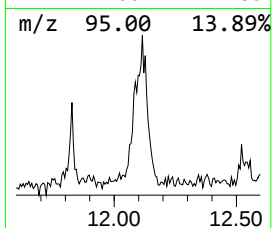
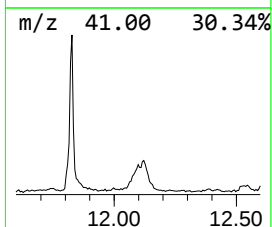
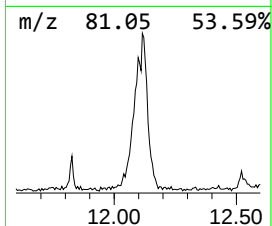
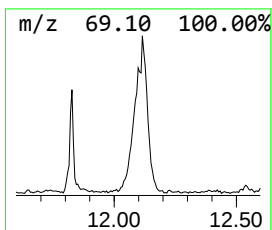
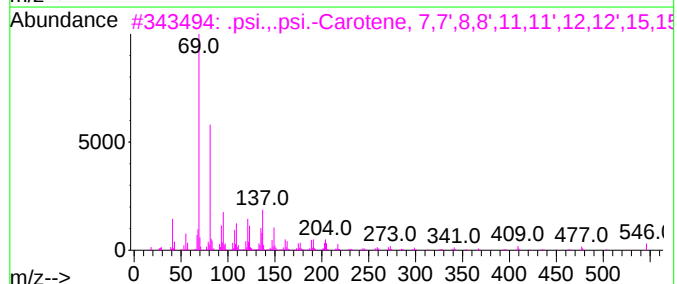
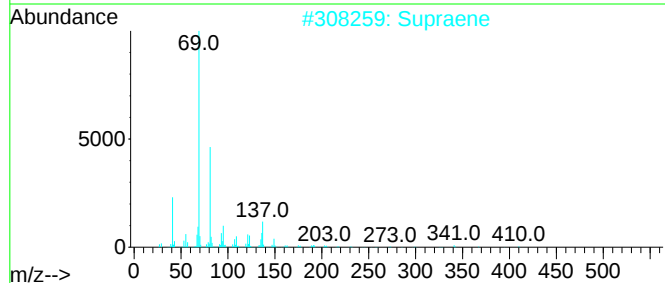
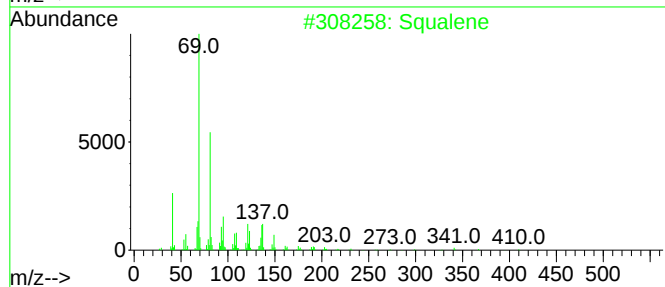
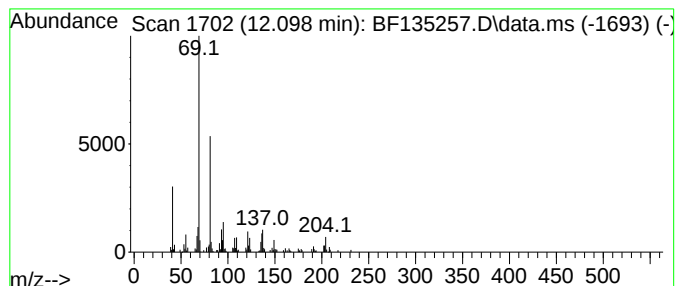
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	3.06 ng	182439	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	90
3			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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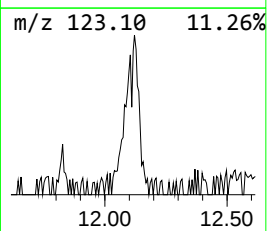
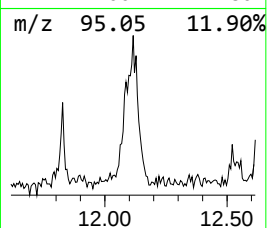
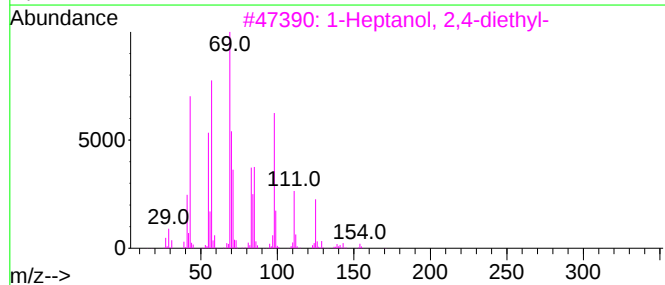
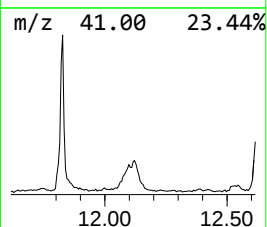
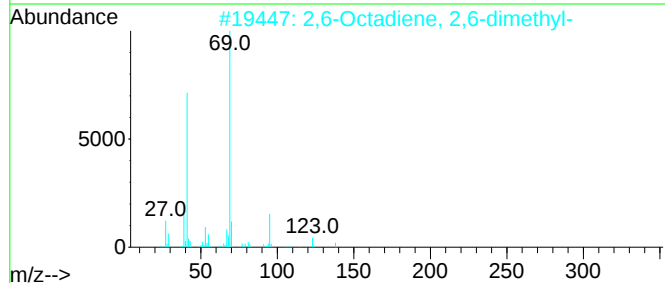
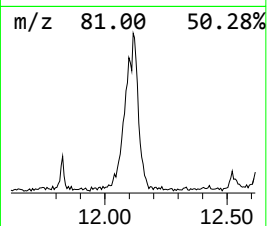
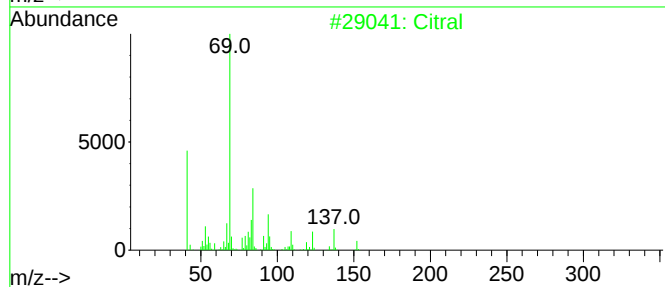
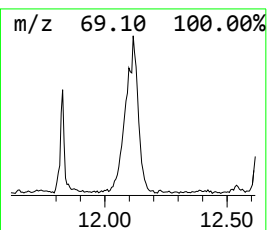
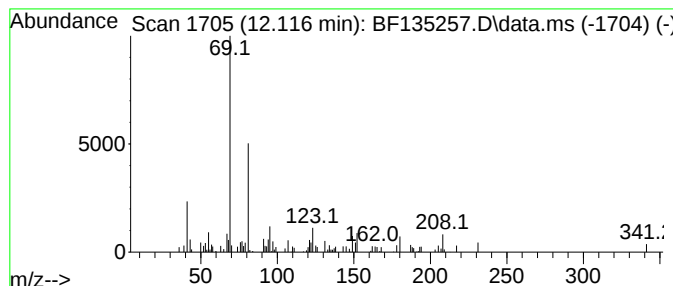
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Peak Number 4 Citral Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.116	3.12 ng	185796	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Citral	152	C10H16O	005392-40-5	64
2			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53
3			1-Heptanol, 2,4-diethyl-	172	C11H24O	080192-55-8	47
4			Squalene	410	C30H50	000111-02-4	45
5			1-(3,5-Dinitrophenoxy)-3,7,11-tr...	388	C21H28N2O5	1000187-44-2	45



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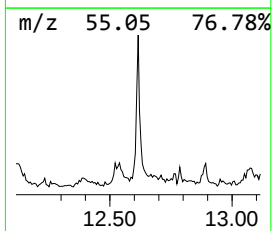
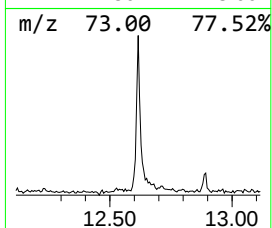
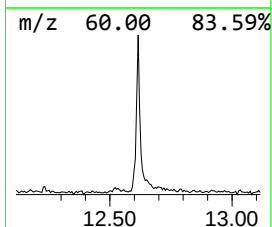
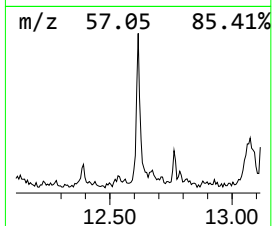
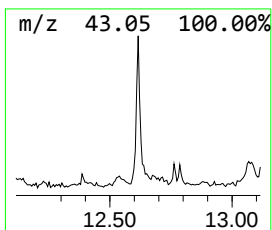
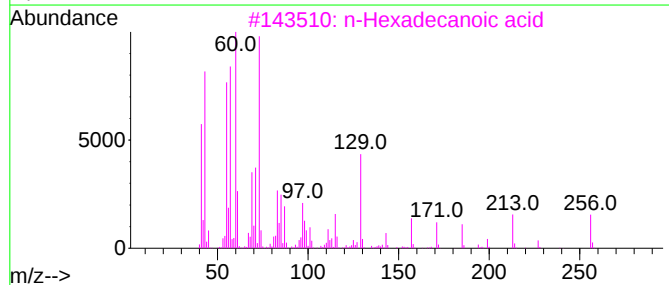
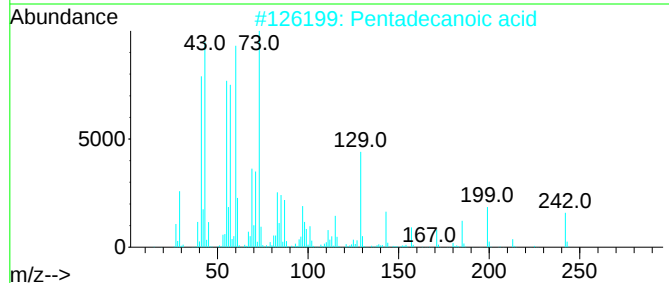
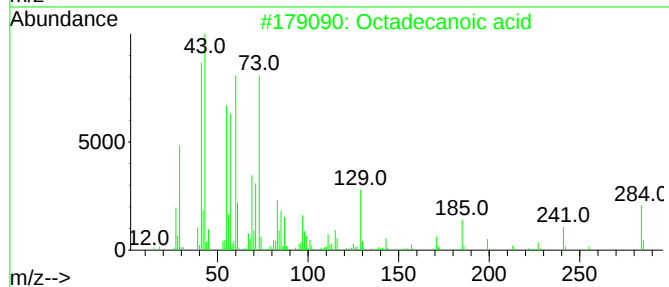
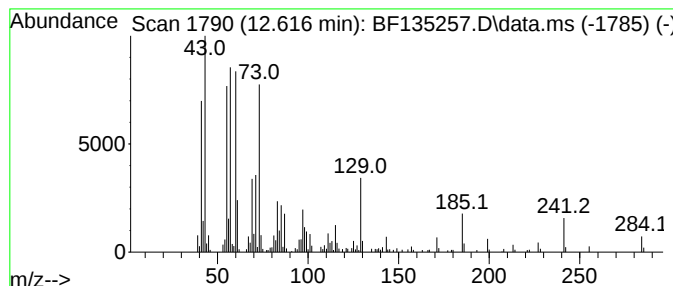
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	6.12 ng	223885	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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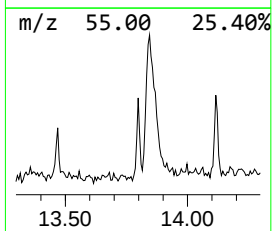
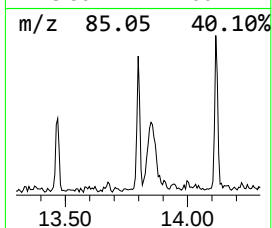
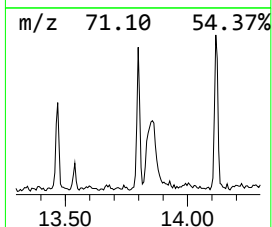
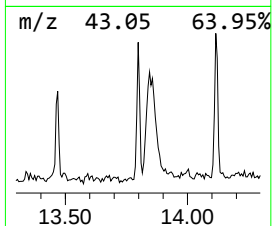
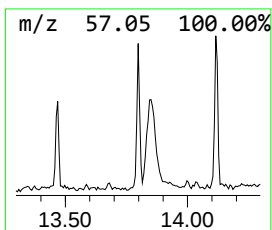
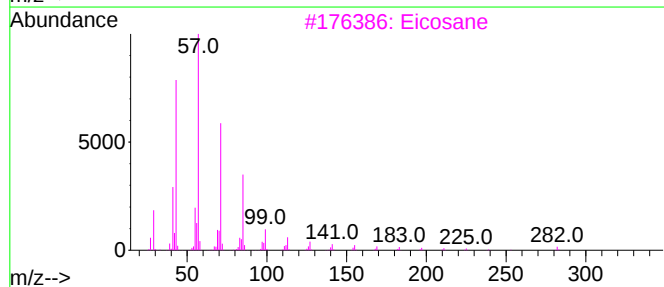
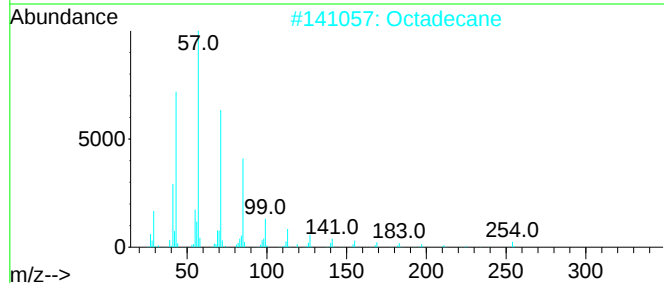
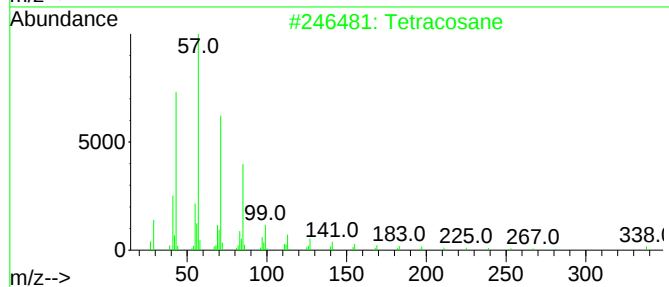
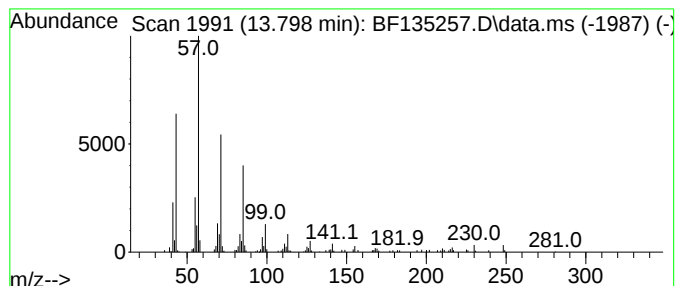
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.66 ng	97372	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Octadecane	254	C18H38	000593-45-3	87
3			Eicosane	282	C20H42	000112-95-8	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135257.D
Acq On : 14 Sep 2023 16:49
Operator : CG\JU
Sample : 04338-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

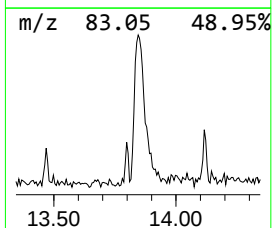
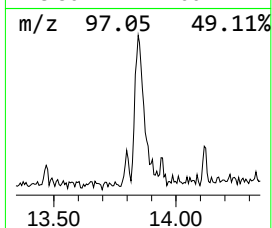
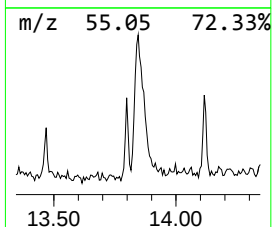
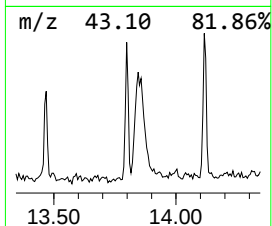
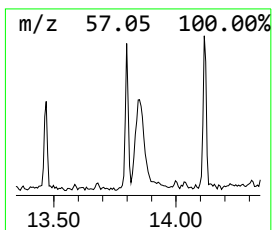
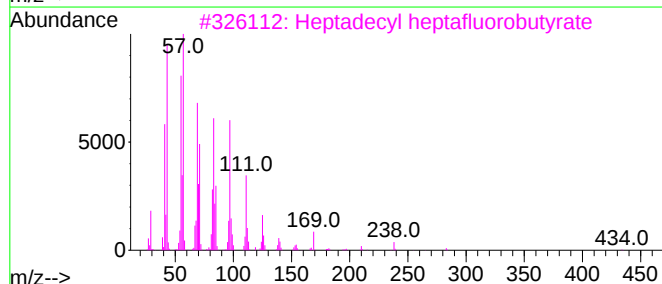
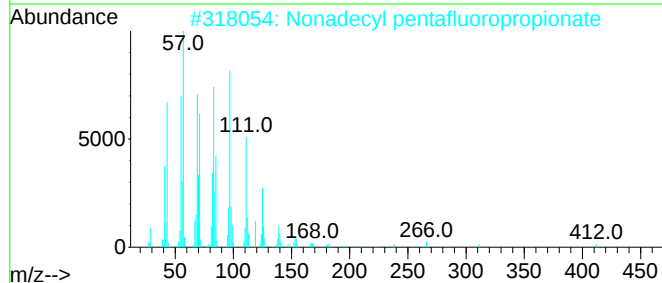
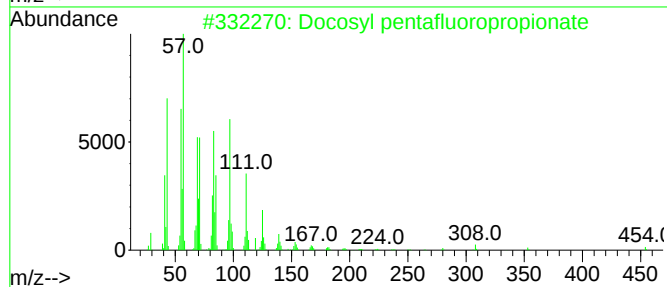
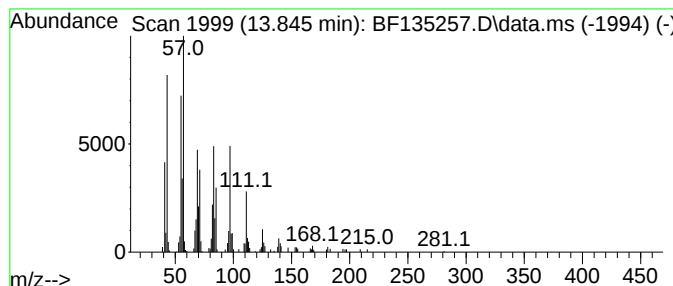
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosyl pentafluoropropionate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	7.74 ng	283054	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135257.D
Acq On : 14 Sep 2023 16:49
Operator : CG\JU
Sample : 04338-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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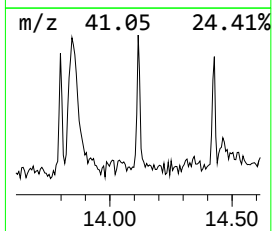
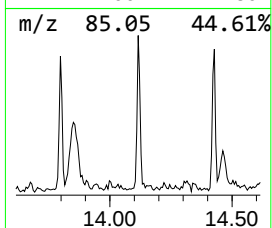
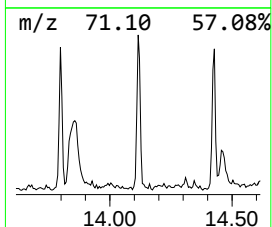
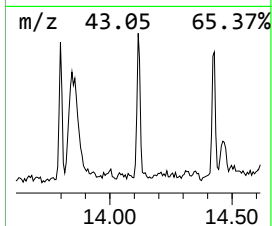
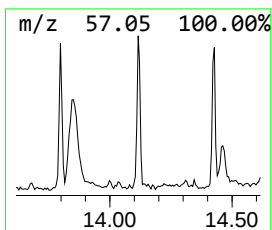
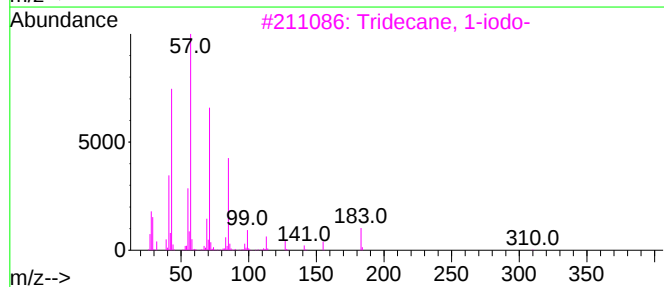
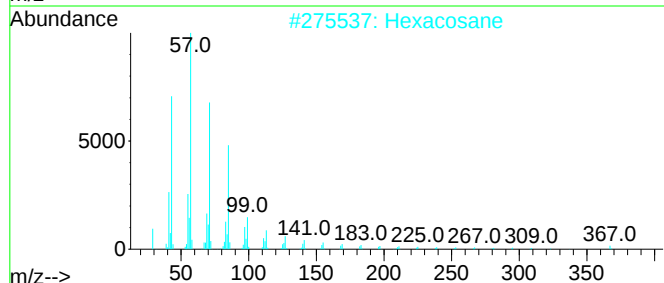
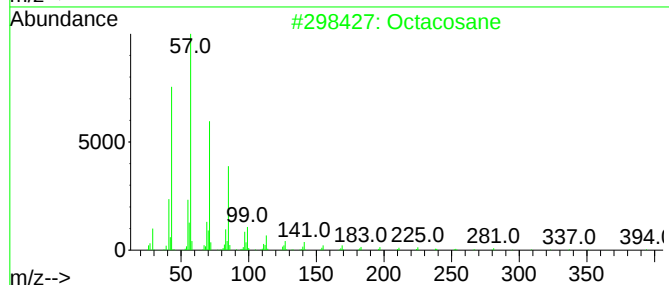
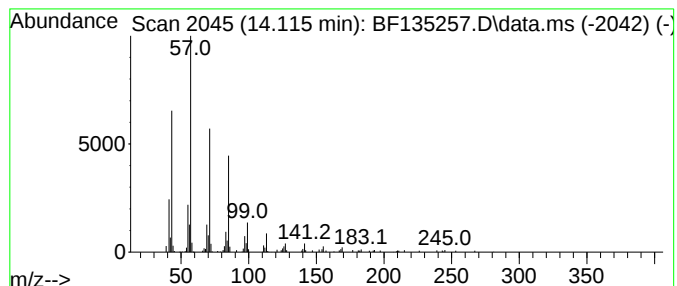
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.116	2.76 ng	100899	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
4			Hexadecane	226	C16H34	000544-76-3	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135257.D
Acq On : 14 Sep 2023 16:49
Operator : CG\JU
Sample : 04338-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

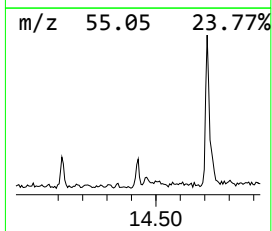
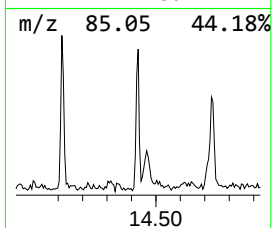
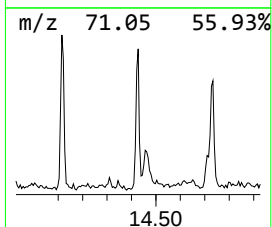
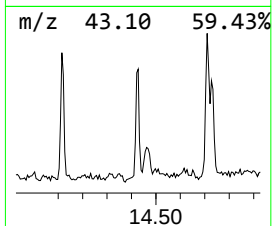
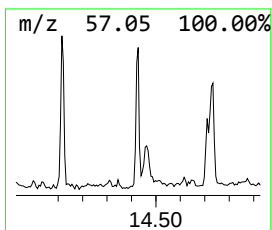
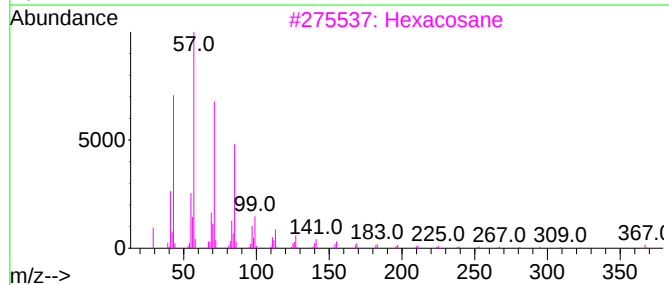
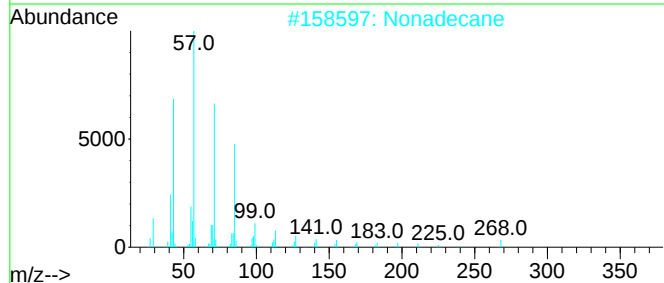
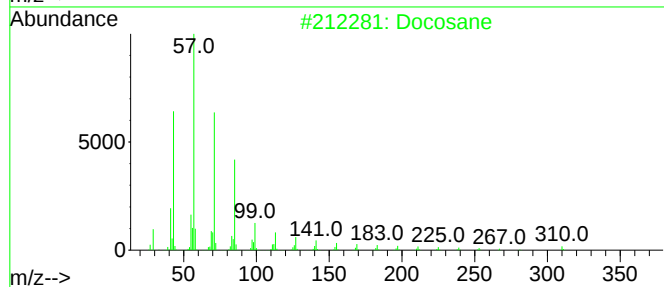
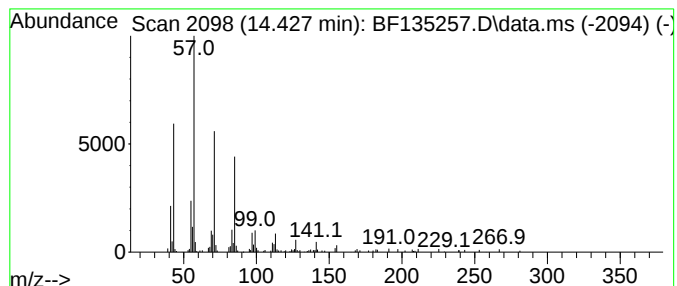
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	2.57 ng	93804	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	87
2			Nonadecane	268	C19H40	000629-92-5	83
3			Hexacosane	366	C26H54	000630-01-3	76
4			Hentriacontane	437	C31H64	000630-04-6	74
5			Heptacosane	380	C27H56	000593-49-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135257.D
Acq On : 14 Sep 2023 16:49
Operator : CG\JU
Sample : 04338-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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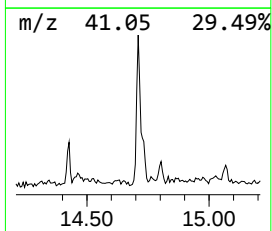
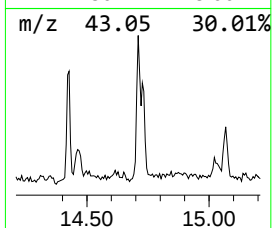
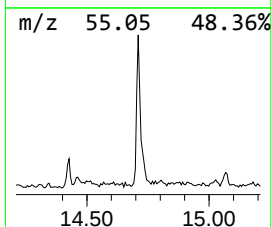
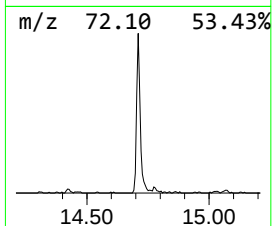
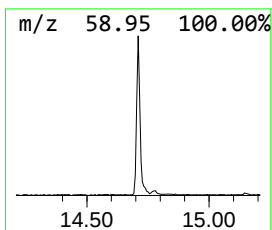
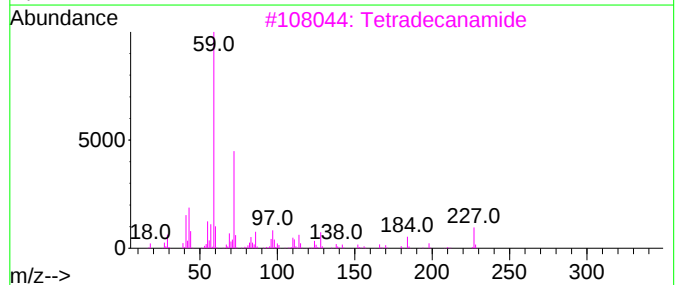
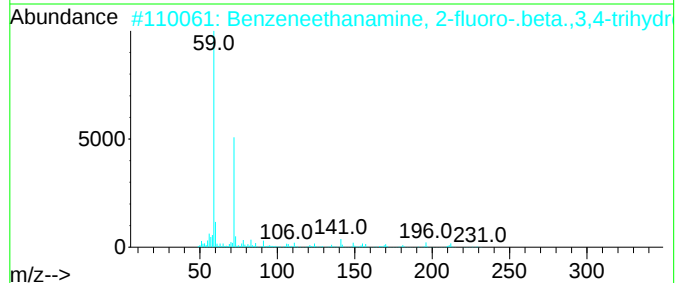
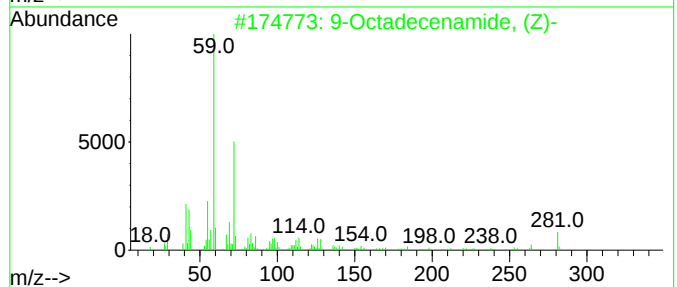
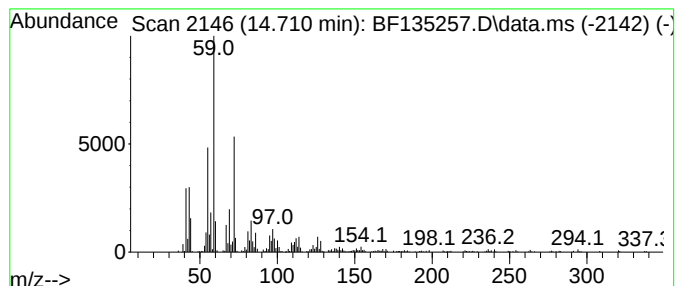
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	12.75 ng	447831	Perylene-d12	15.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	83
3		Tetradecanamide	227	C14H29NO	000638-58-4	78
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
5		Hexadecanamide	255	C16H33NO	000629-54-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091423\
Data File : BF135257.D
Acq On : 14 Sep 2023 16:49
Operator : CG\JU
Sample : 04338-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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-...	5.028	4.0	ng	152169	1	6.763	767981	20.0
n-Hexadecanoic ...	11.827	11.9	ng	707056	4	11.286	1192120	20.0
Squalene	12.098	3.1	ng	182439	4	11.286	1192120	20.0
Citral	12.116	3.1	ng	185796	4	11.286	1192120	20.0
Octadecanoic acid	12.616	6.1	ng	223885	5	13.945	731146	20.0
Tetracosane	13.798	2.7	ng	97372	5	13.945	731146	20.0
Docosyl pentafl...	13.845	7.7	ng	283054	5	13.945	731146	20.0
Octacosane	14.116	2.8	ng	100899	5	13.945	731146	20.0
Docosane	14.427	2.6	ng	93804	5	13.945	731146	20.0
9-Octadecenamid...	14.710	12.8	ng	447831	6	15.410	702598	20.0