

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128548.D
 Acq On : 28 May 2022 15:05
 Operator : CG\JU
 Sample : N2931-15
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P016-SS001-0612-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	3	5	15	rVB	82657	88286	1.14%	0.170%
2	5.092	473	477	487	rVB	186031	307404	3.97%	0.590%
3	5.469	534	541	544	rBV	5382355	6821033	88.06%	13.096%
4	6.469	704	711	714	rBV	4883168	7097935	91.64%	13.628%
5	6.575	726	729	733	rVB	113684	89167	1.15%	0.171%
6	6.839	770	774	777	rVB	1343885	1163289	15.02%	2.233%
7	7.404	863	870	873	rBV	4173449	4872806	62.91%	9.356%
8	8.116	987	991	995	rBV	1682727	1570586	20.28%	3.015%
9	9.198	1169	1175	1179	rBV	6487895	7745532	100.00%	14.871%
10	9.875	1284	1290	1293	rBV	2178455	1808588	23.35%	3.472%
11	10.669	1417	1425	1428	rBV	5056077	5262276	67.94%	10.103%
12	11.363	1539	1543	1546	rBV	2185545	1807713	23.34%	3.471%
13	11.898	1629	1634	1648	rBV	1053054	1114400	14.39%	2.140%
14	12.680	1763	1767	1781	rBV	408925	425740	5.50%	0.817%
15	12.957	1809	1814	1817	rBV	6349608	6911577	89.23%	13.270%
16	13.886	1964	1972	1986	rBV3	355065	1179127	15.22%	2.264%
17	13.998	1987	1991	1995	rVV	1355302	1333939	17.22%	2.561%
18	14.098	2000	2008	2018	rVV	475859	561365	7.25%	1.078%
19	14.174	2018	2021	2025	rVB	123426	105049	1.36%	0.202%
20	14.480	2070	2073	2076	rBV	133622	109789	1.42%	0.211%
21	14.792	2122	2126	2131	rVB	100470	105449	1.36%	0.202%
22	15.127	2180	2183	2190	rVB	100048	116103	1.50%	0.223%
23	15.462	2235	2240	2245	rBV	857342	1033410	13.34%	1.984%
24	15.509	2245	2248	2256	rVB	61079	82230	1.06%	0.158%
25	15.951	2319	2323	2330	rVB	57724	84463	1.09%	0.162%
26	16.092	2338	2347	2349	rBV8	55691	137361	1.77%	0.264%
27	18.603	2769	2774	2785	rVB3	59448	149834	1.93%	0.288%

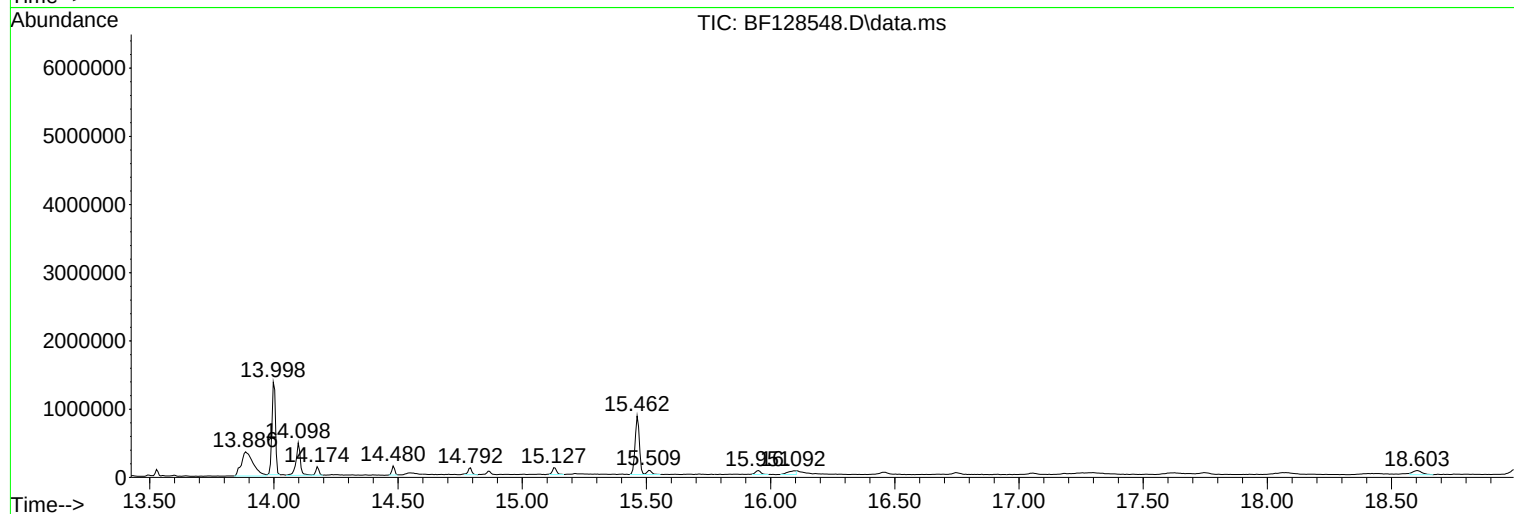
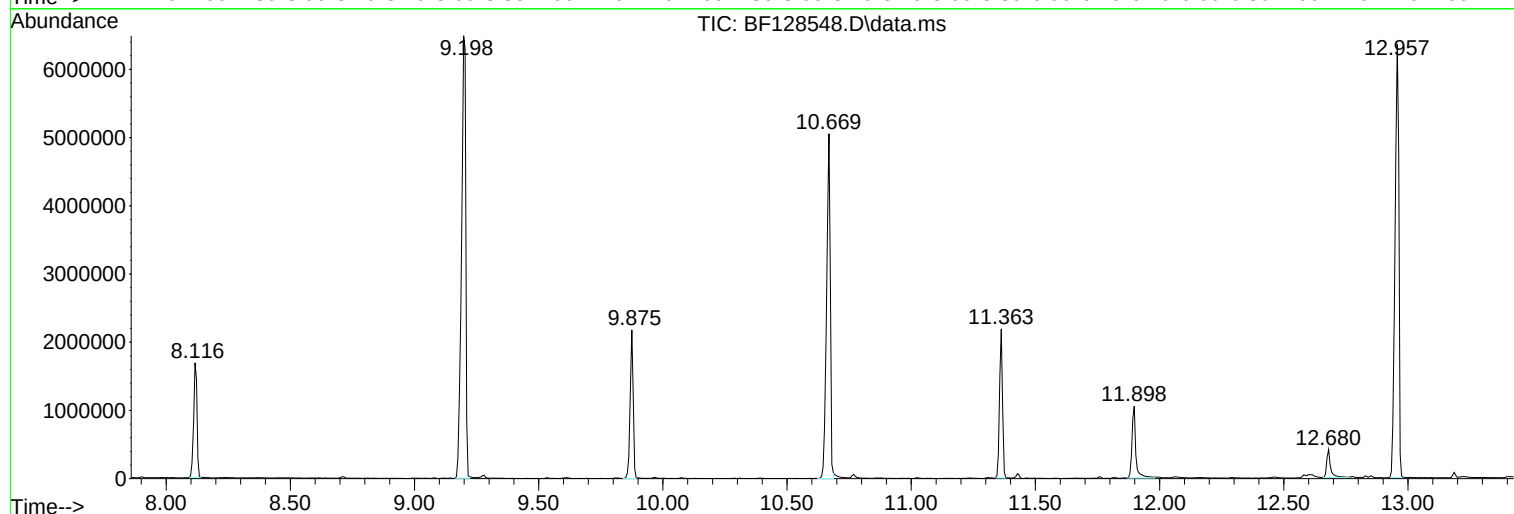
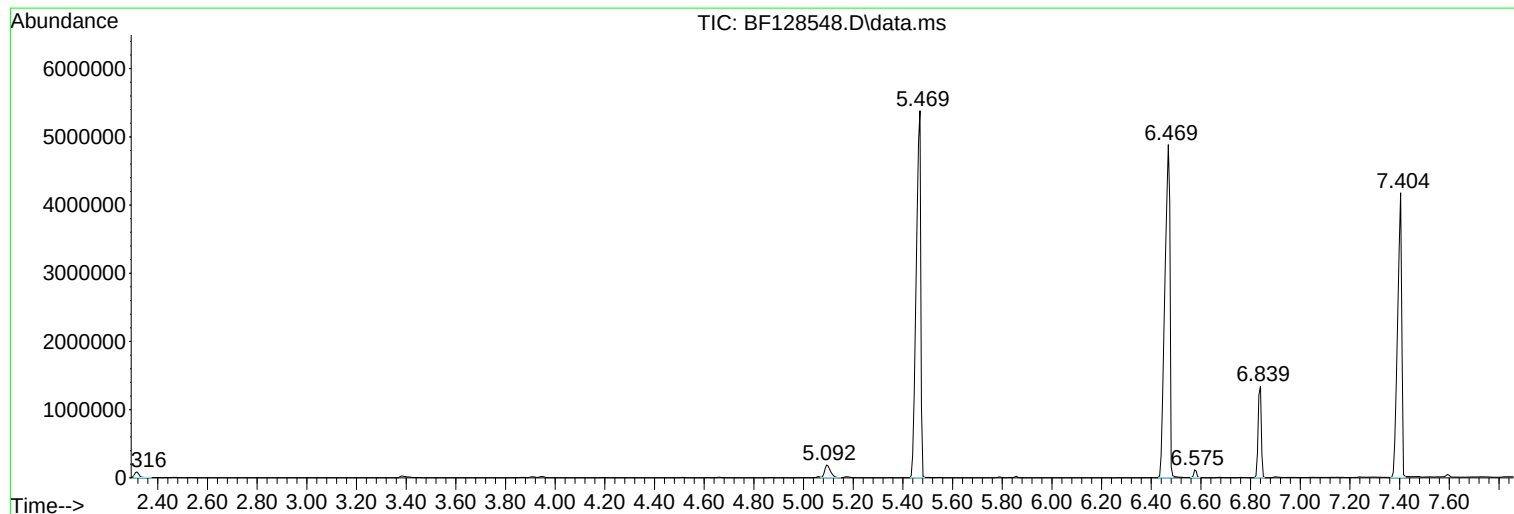
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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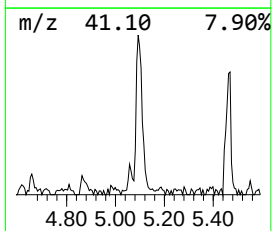
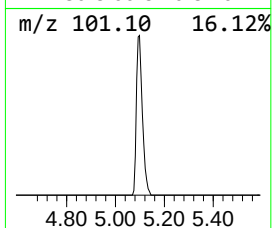
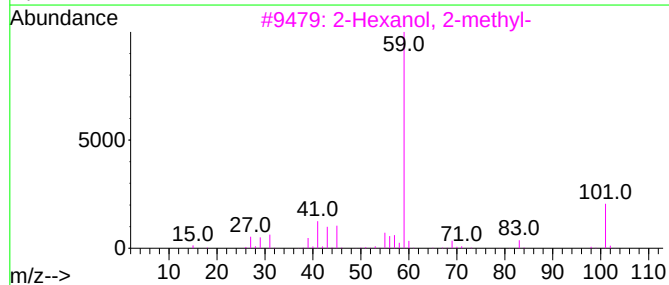
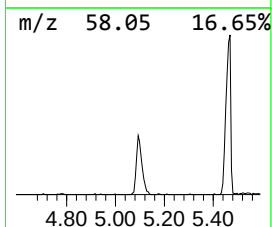
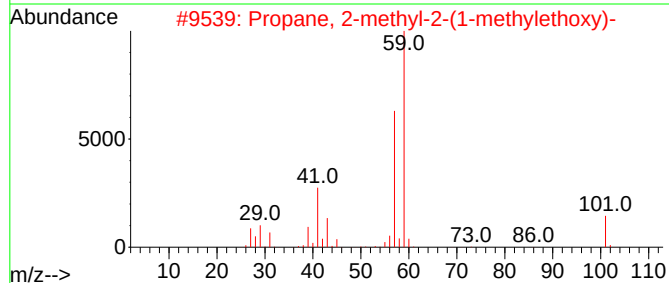
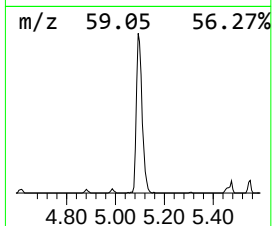
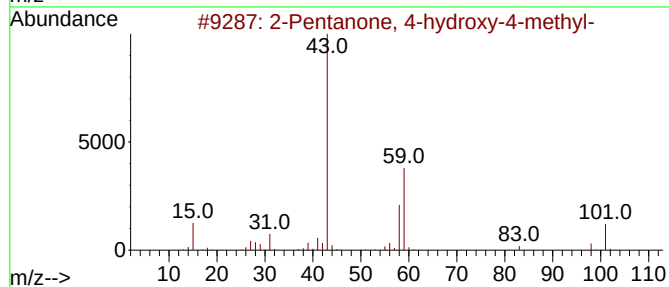
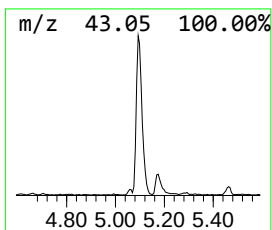
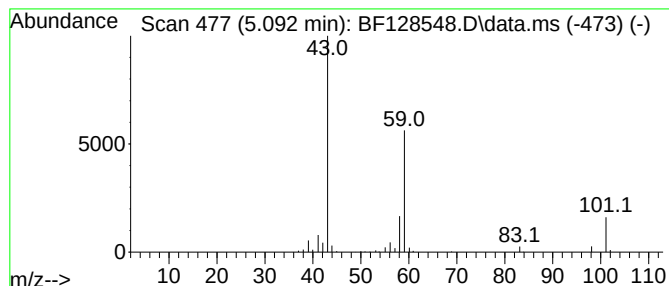
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	5.29 ng	307404	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		



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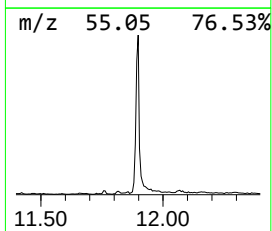
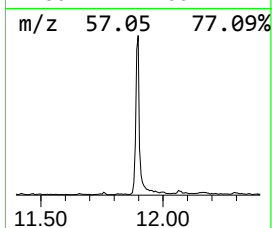
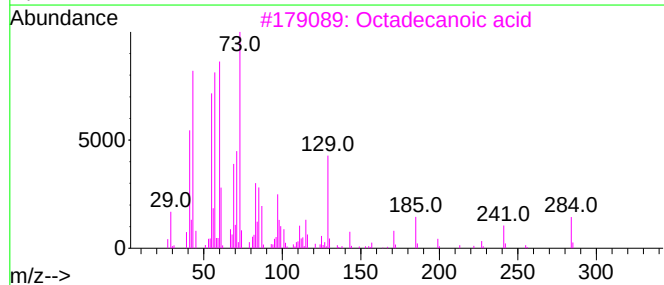
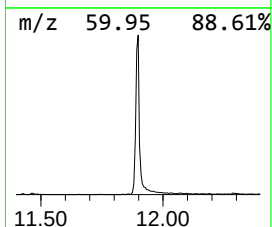
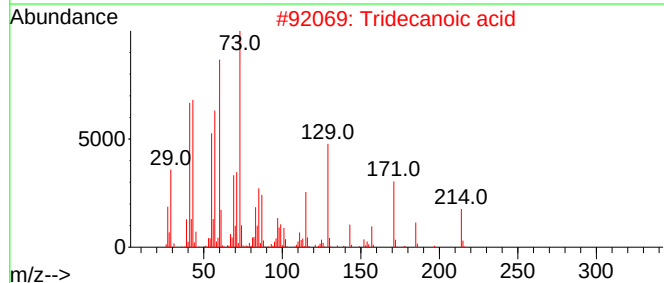
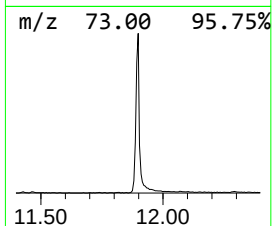
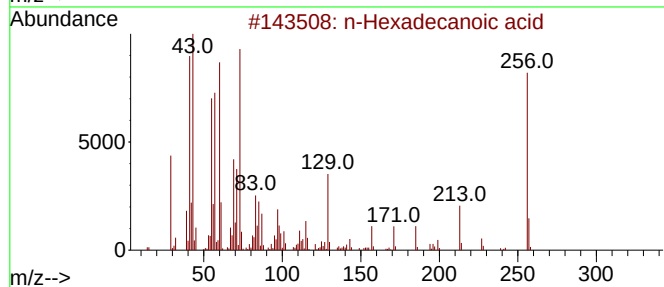
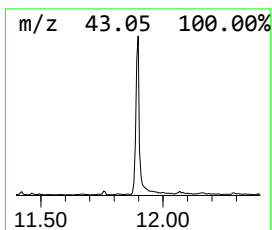
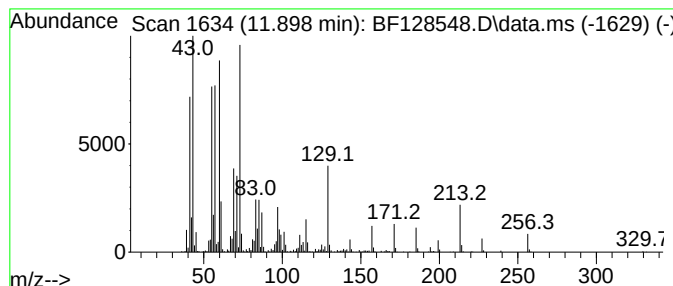
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	12.33 ng	1114400	Phenanthrene-d10	11.363

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	93
3		Octadecanoic acid	284	C18H36O2	000057-11-4	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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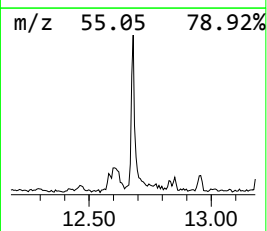
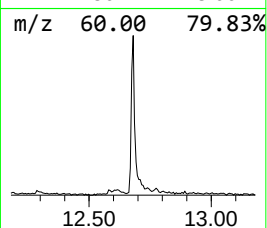
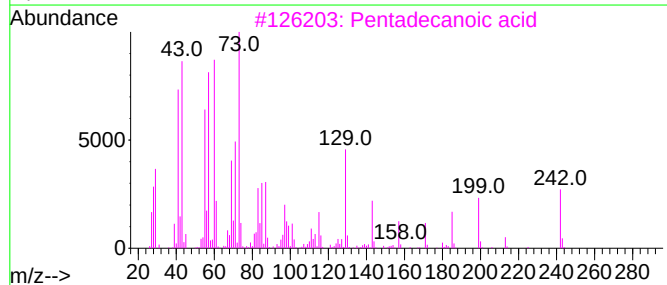
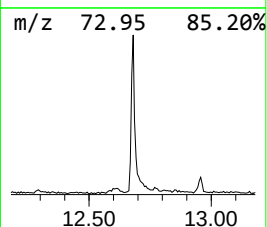
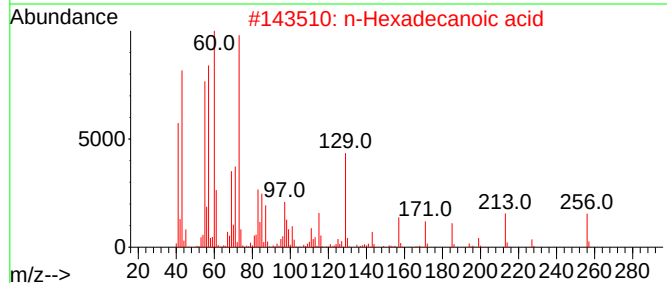
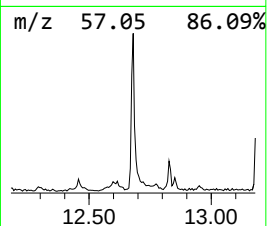
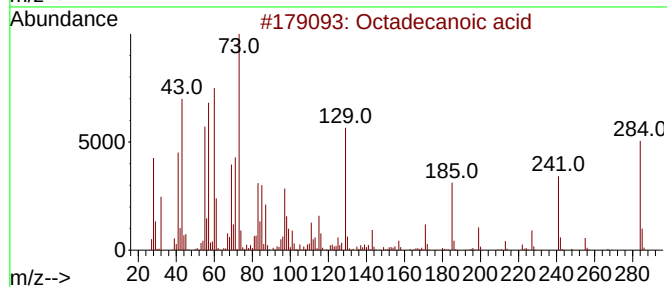
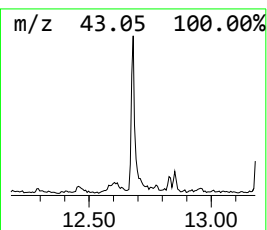
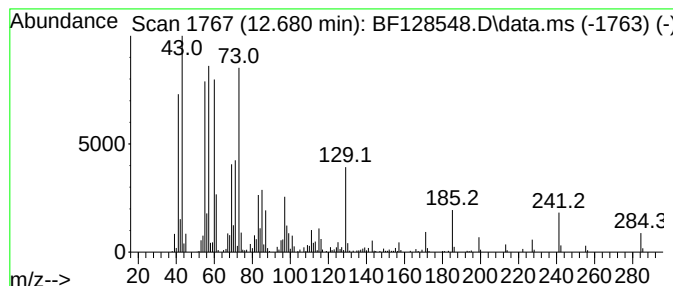
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	4.71 ng	425740	Phenanthrene-d10	11.363

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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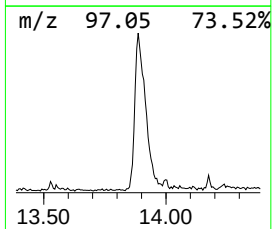
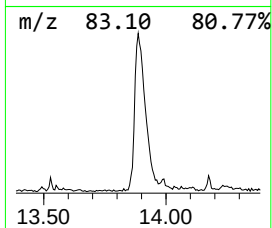
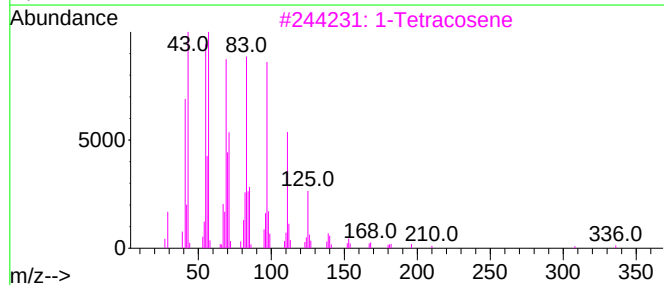
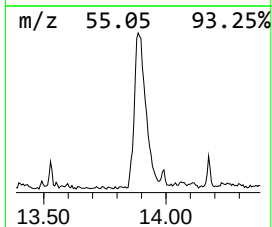
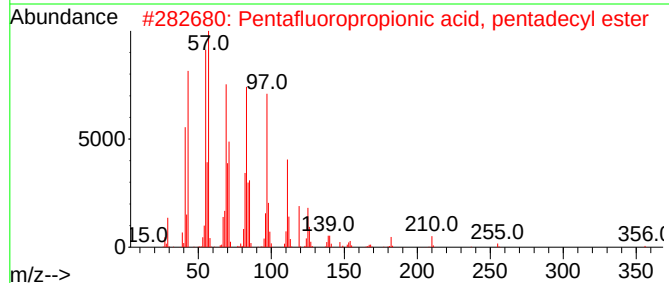
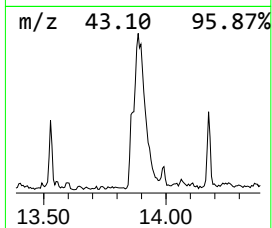
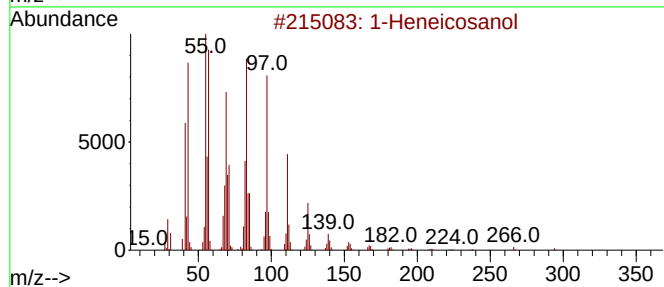
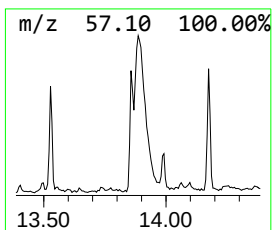
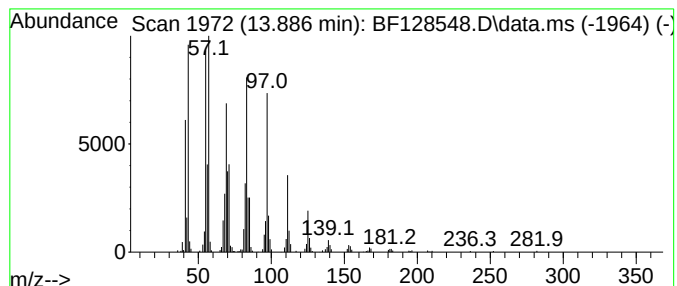
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Peak Number 4 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	17.68 ng	1179130	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			1-Tetracosene	336	C24H48	010192-32-2	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Cyclotetradecane	196	C14H28	000295-17-0	93



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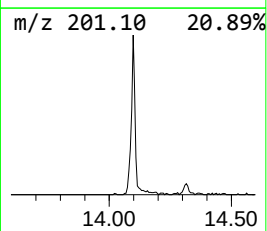
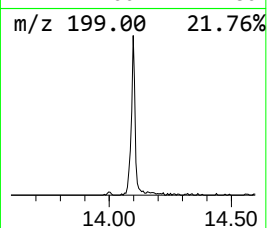
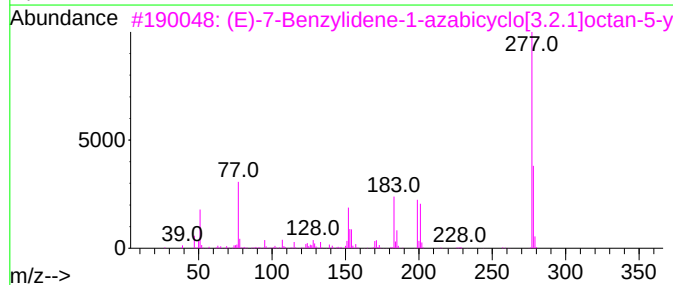
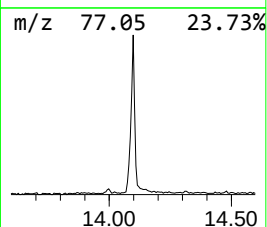
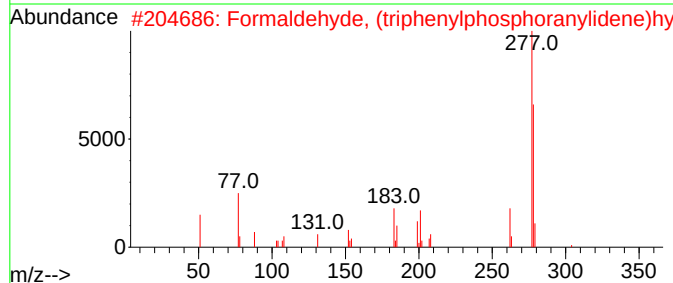
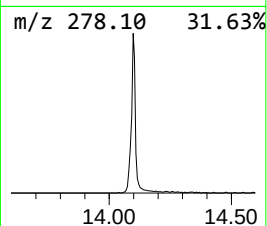
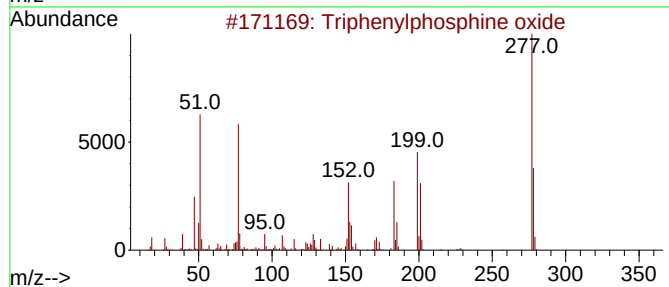
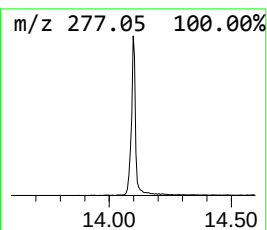
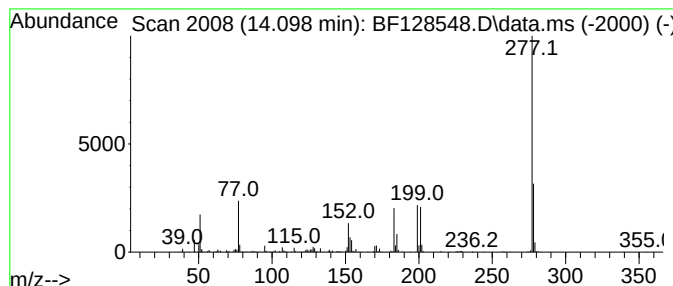
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	8.42 ng	561365	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38



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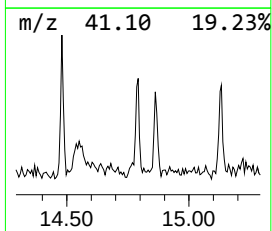
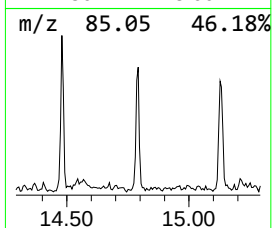
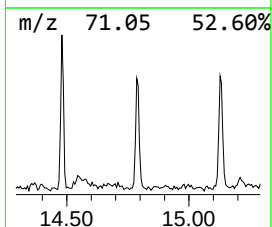
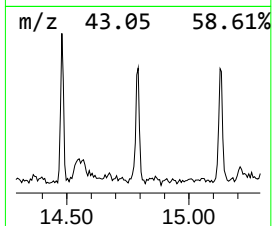
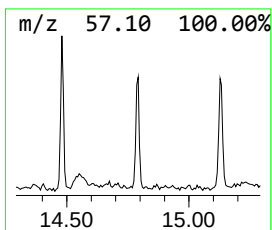
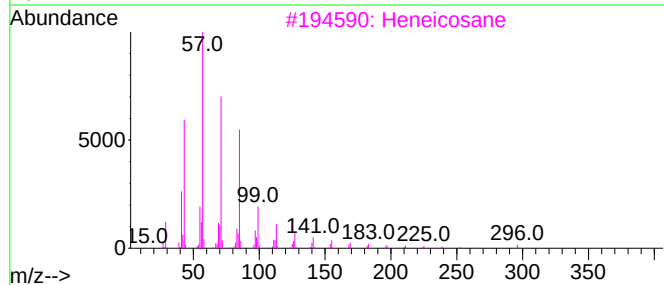
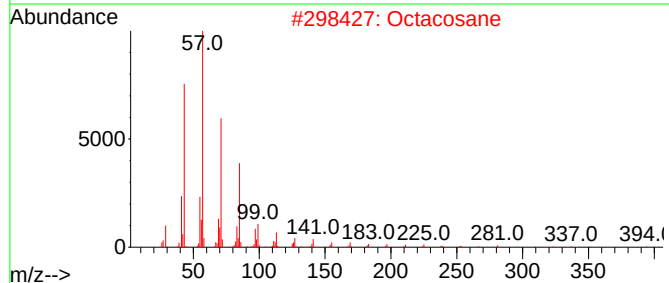
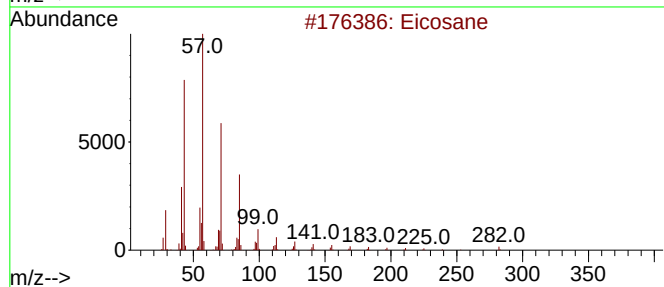
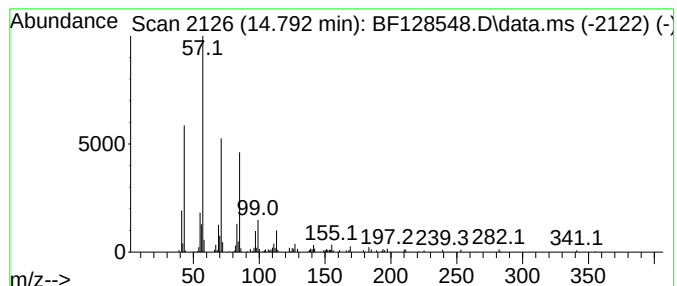
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	2.04 ng	105449	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heptadecane	240	C17H36	000629-78-7	86
5			Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128548.D
Acq On : 28 May 2022 15:05
Operator : CG\JU
Sample : N2931-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P016-SS001-0612-01

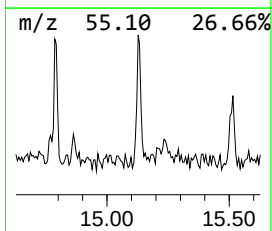
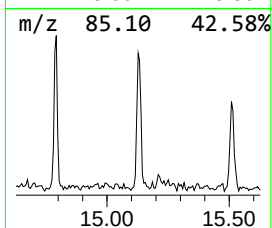
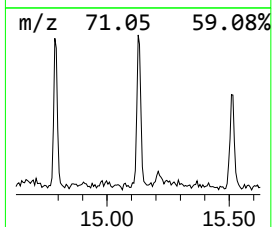
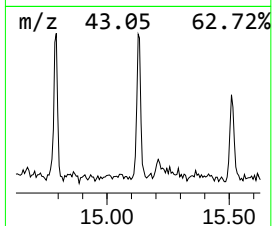
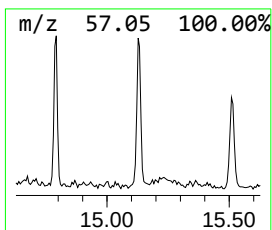
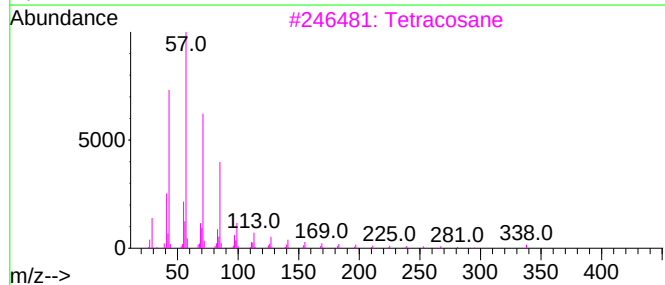
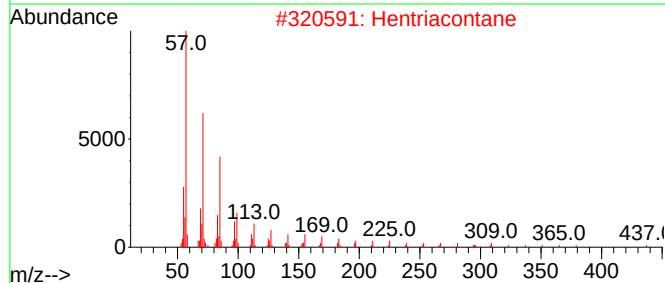
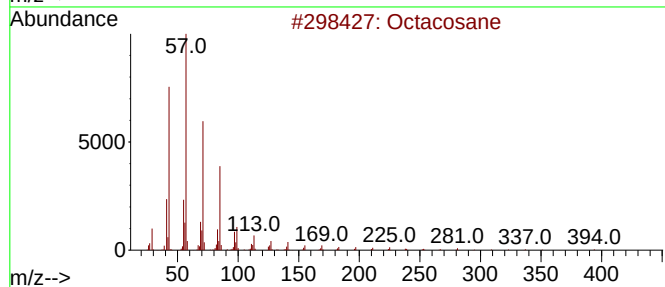
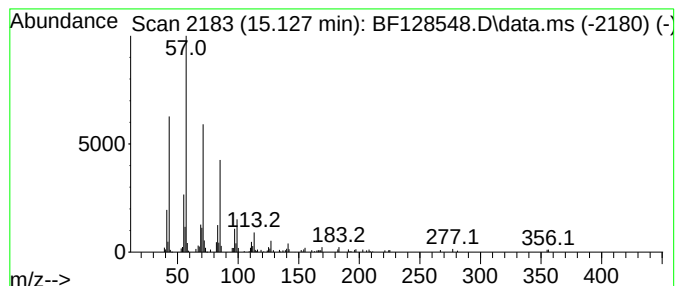
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.25 ng	116103	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Hentriacontane	437	C31H64	000630-04-6	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128548.D
Acq On : 28 May 2022 15:05
Operator : CG\JU
Sample : N2931-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P016-SS001-0612-01

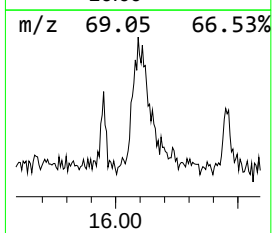
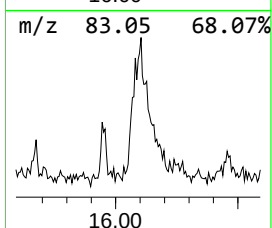
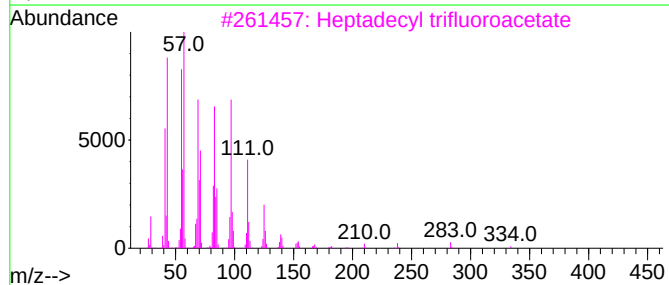
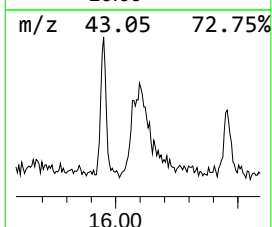
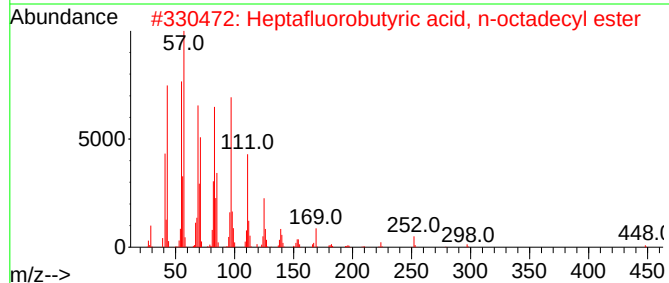
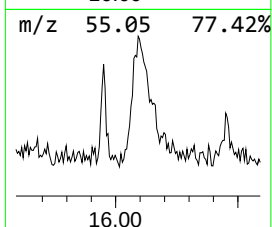
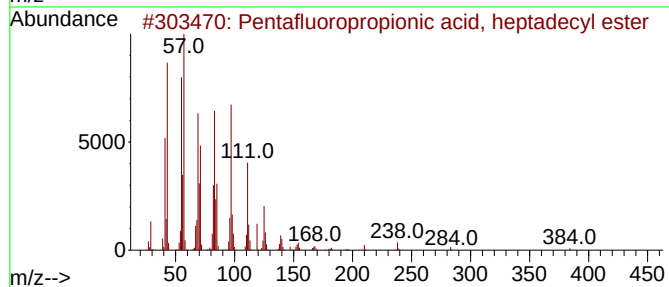
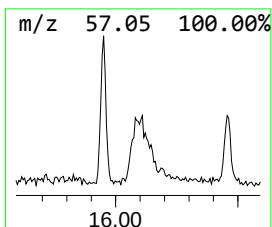
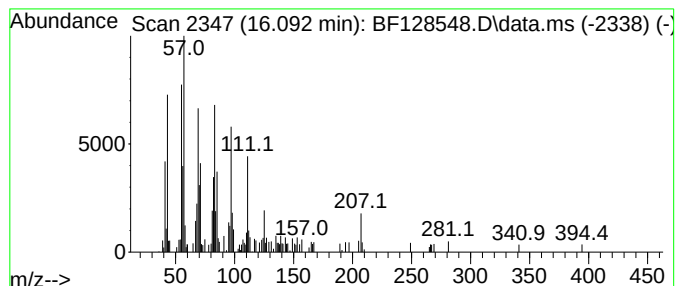
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	2.66 ng	137361	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128548.D
Acq On : 28 May 2022 15:05
Operator : CG\JU
Sample : N2931-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P016-SS001-0612-01

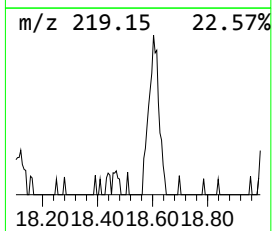
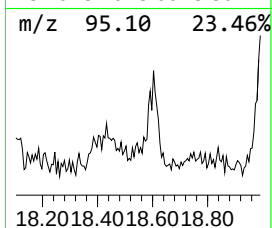
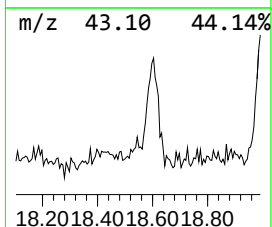
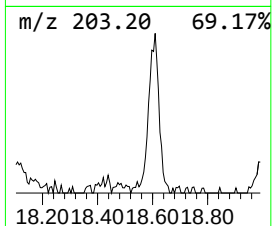
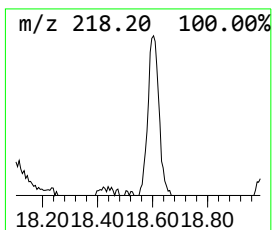
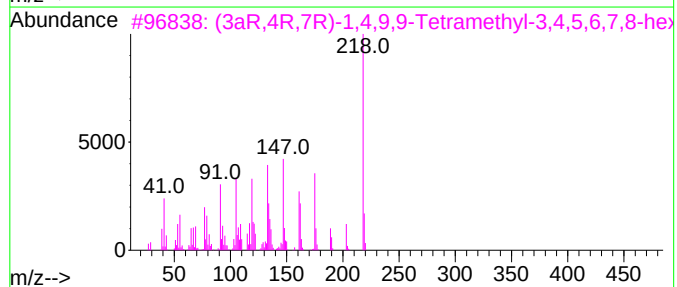
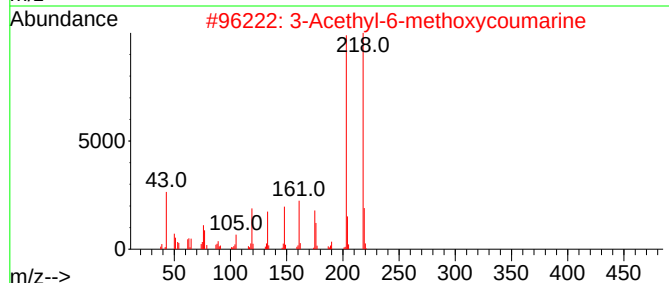
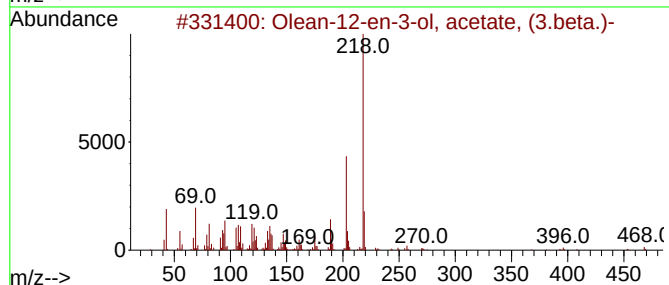
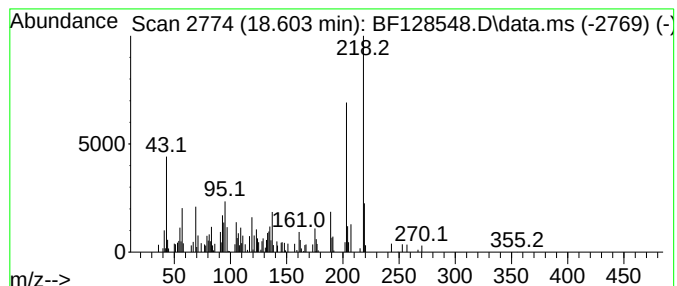
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Olean-12-en-3-ol, acetate, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.603	2.90 ng	149834	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	80
2			3-Acethyl-6-methoxycoumarine	218	C12H10O4	013252-80-7	68
3			(3aR,4R,7R)-1,4,9,9-Tetramethyl-...	218	C15H22O	003466-15-7	60
4			Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	58
5			2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128548.D
Acq On : 28 May 2022 15:05
Operator : CG\JU
Sample : N2931-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P016-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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-...	5.092	5.3	ng	307404	1	6.839	1163290	20.0
n-Hexadecanoic ...	11.898	12.3	ng	1114400	4	11.363	1807710	20.0
Octadecanoic acid	12.680	4.7	ng	425740	4	11.363	1807710	20.0
1-Heneicosanol	13.886	17.7	ng	1179130	5	13.998	1333940	20.0
Triphenylphosph...	14.098	8.4	ng	561365	5	13.998	1333940	20.0
Eicosane	14.792	2.0	ng	105449	6	15.462	1033410	20.0
Octacosane	15.127	2.3	ng	116103	6	15.462	1033410	20.0
Pentafluoroprop...	16.092	2.7	ng	137361	6	15.462	1033410	20.0
Olean-12-en-3-o...	18.603	2.9	ng	149834	6	15.462	1033410	20.0