

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128549.D
 Acq On : 28 May 2022 15:35
 Operator : CG\JU
 Sample : N2933-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P023-SS001-1218-01

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: BF128549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.346	177	180	192	rBV	29503	67886	1.12%	0.170%
2	5.075	470	474	481	rVB	184279	243374	4.02%	0.609%
3	5.463	533	540	543	rBV	4212953	4860274	80.37%	12.159%
4	6.463	704	710	713	rBV	4076961	5018455	82.99%	12.554%
5	6.575	727	729	735	rVB	110509	79921	1.32%	0.200%
6	6.834	770	773	777	rBV	1299029	1122585	18.56%	2.808%
7	7.398	863	869	872	rBV	3117821	3481403	57.57%	8.709%
8	8.116	987	991	995	rBV	1625352	1508591	24.95%	3.774%
9	9.198	1169	1175	1178	rBV	5947726	6047024	100.00%	15.128%
10	9.875	1284	1290	1293	rBV	2098050	1740400	28.78%	4.354%
11	10.663	1418	1424	1428	rBV	3516346	3816672	63.12%	9.548%
12	10.769	1438	1442	1453	rVB	281287	245567	4.06%	0.614%
13	11.363	1539	1543	1546	rBV	2131175	1761913	29.14%	4.408%
14	11.757	1607	1610	1614	rVB	143559	119169	1.97%	0.298%
15	11.892	1629	1633	1637	rBV	219487	229972	3.80%	0.575%
16	12.469	1724	1731	1734	rBV3	56451	61749	1.02%	0.154%
17	12.569	1742	1748	1751	rBV4	50180	95793	1.58%	0.240%
18	12.674	1763	1766	1780	rVB2	77498	96627	1.60%	0.242%
19	12.957	1809	1814	1817	rBV	5471765	5519944	91.28%	13.809%
20	13.904	1969	1975	1987	rBV3	86655	241488	3.99%	0.604%
21	13.998	1987	1991	1995	rVV	1264742	1216112	20.11%	3.042%
22	14.098	2001	2008	2013	rBV	508585	558620	9.24%	1.397%
23	14.868	2135	2139	2143	rVB	65602	71819	1.19%	0.180%
24	15.127	2179	2183	2187	rBV	84085	99138	1.64%	0.248%
25	15.463	2235	2240	2245	rBV2	788644	985627	16.30%	2.466%
26	15.951	2318	2323	2333	rVB	135192	202787	3.35%	0.507%
27	16.098	2340	2348	2354	rBV10	30077	112119	1.85%	0.280%
28	17.057	2505	2511	2517	rBV2	58742	121554	2.01%	0.304%
29	17.286	2545	2550	2558	rVB7	82279	177913	2.94%	0.445%
30	18.192	2699	2704	2712	rVB7	28471	68999	1.14%	0.173%

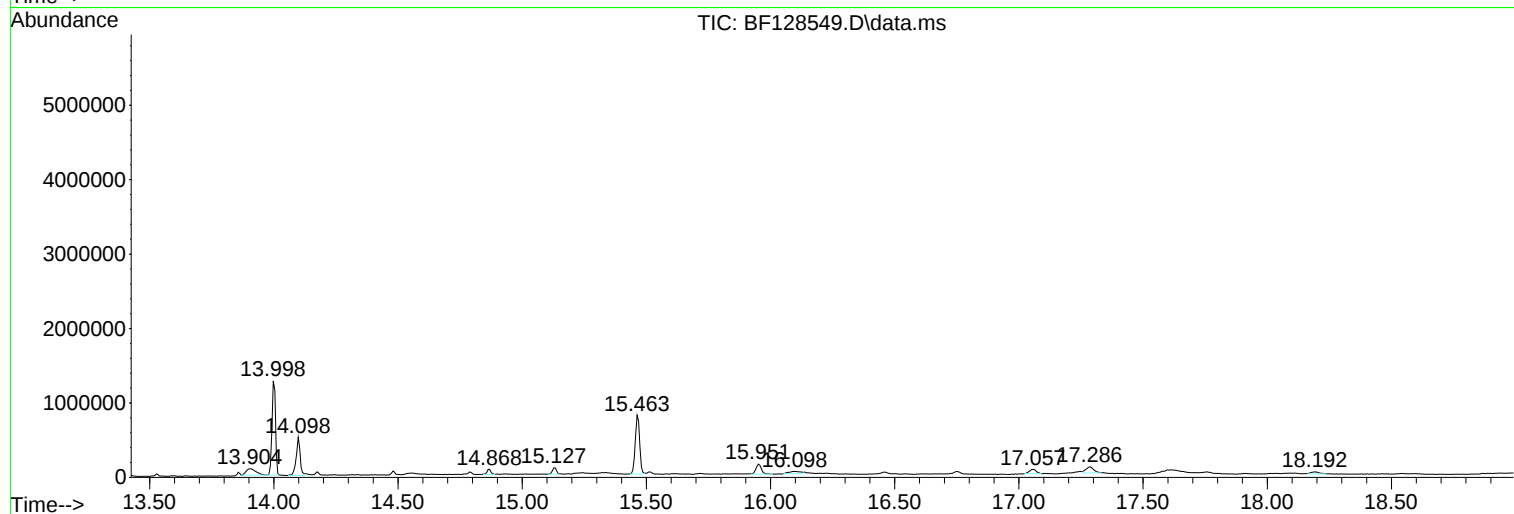
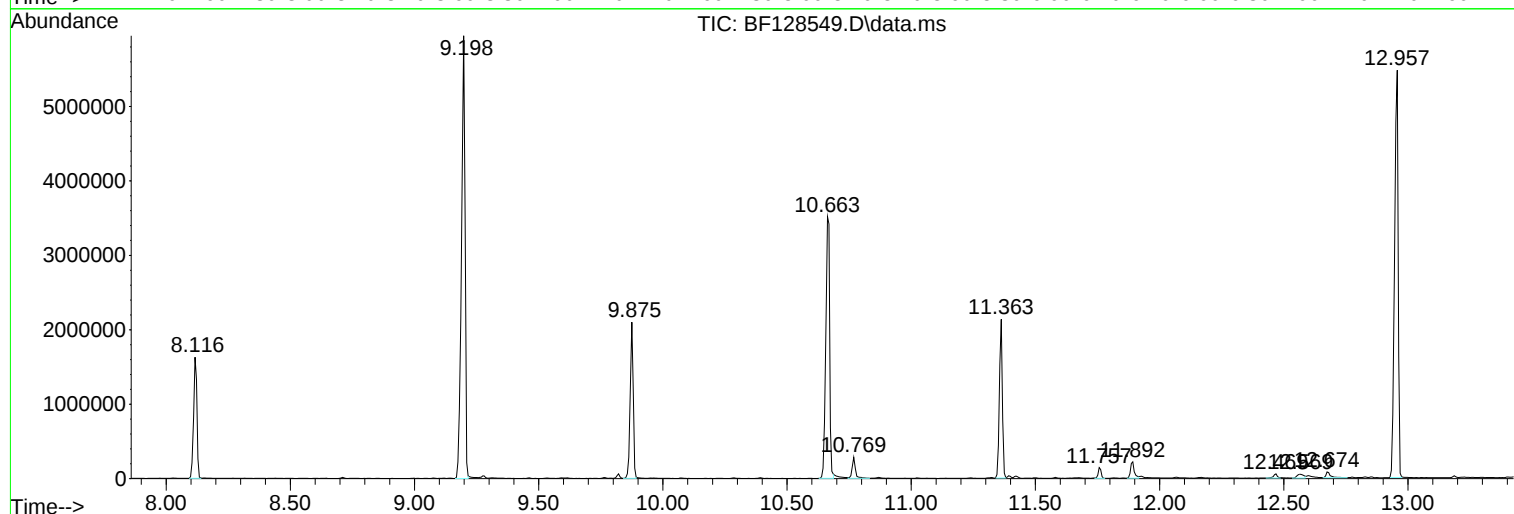
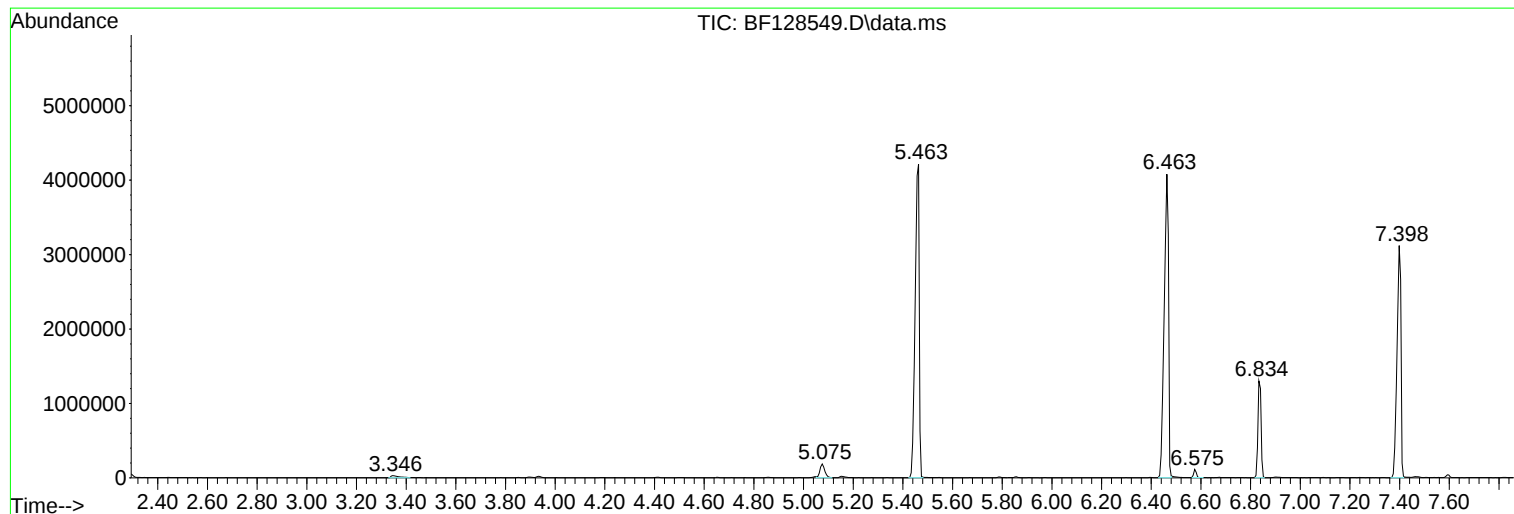
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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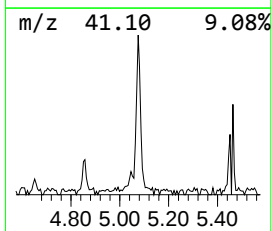
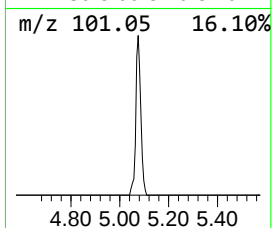
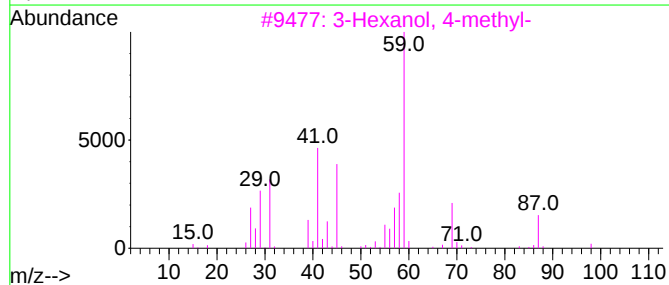
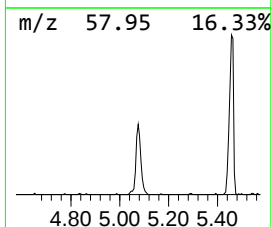
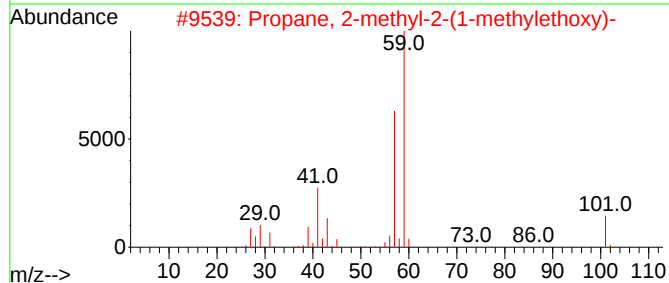
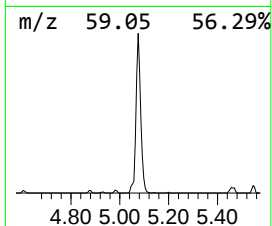
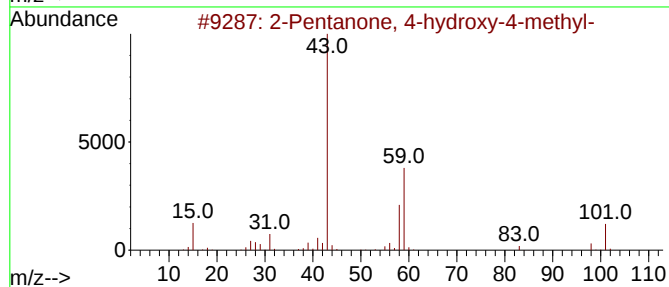
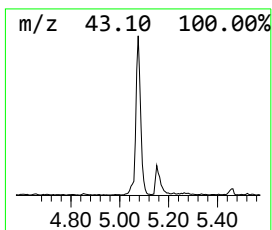
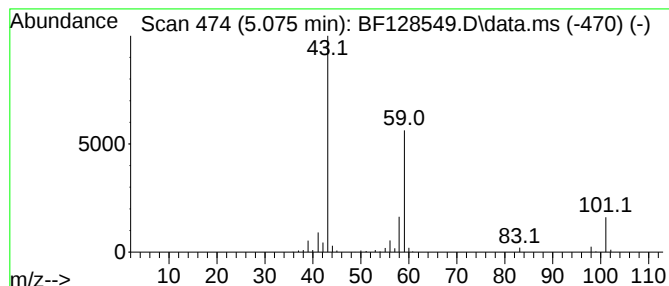
Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.075	4.34 ng	243374	1,4-Dichlorobenzene-d4			6.840
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	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23



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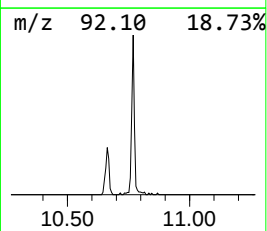
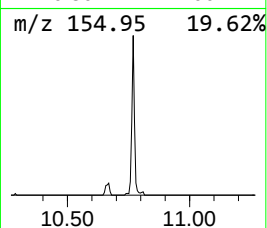
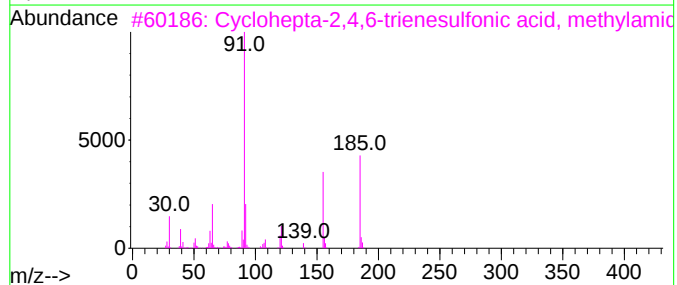
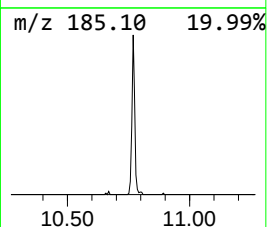
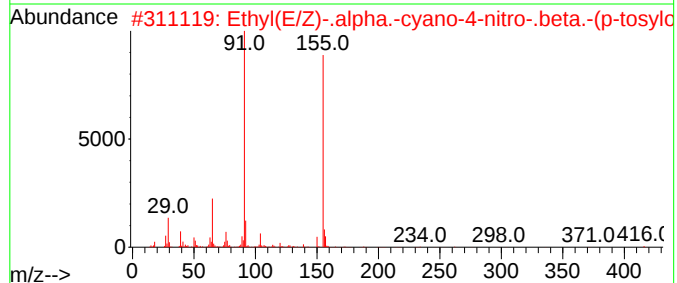
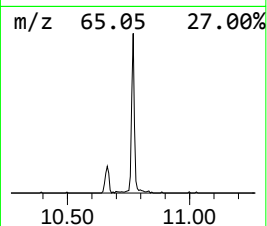
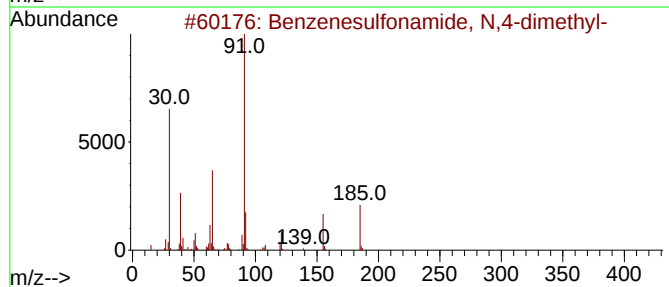
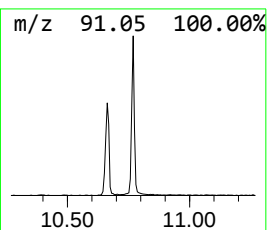
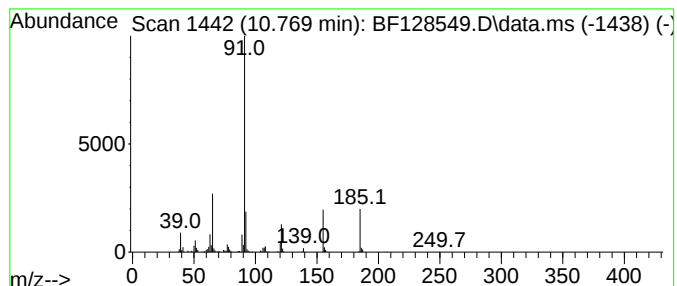
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	2.79 ng	245567	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2			Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
3			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	52
4			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
5			Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	43



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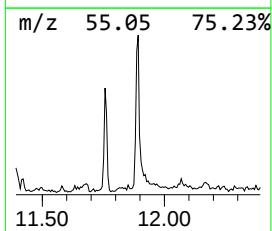
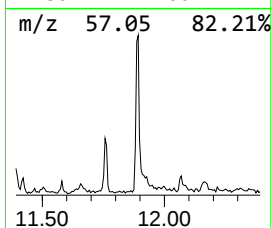
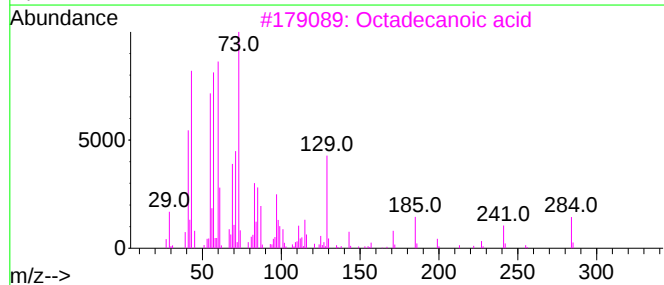
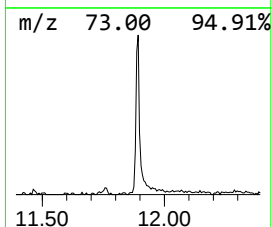
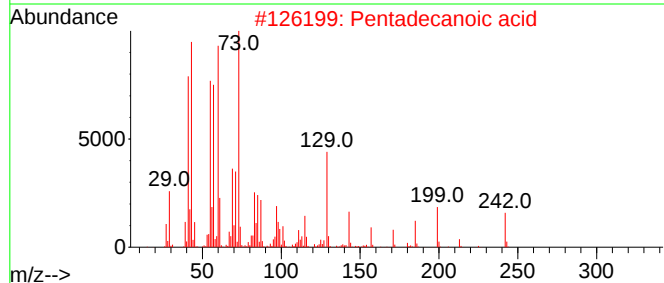
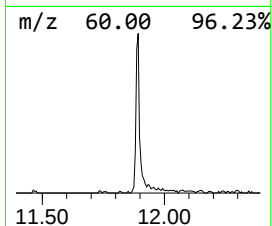
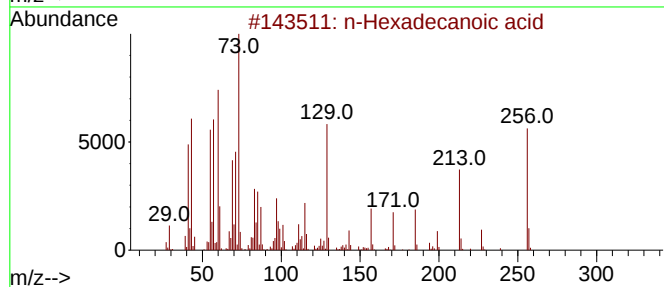
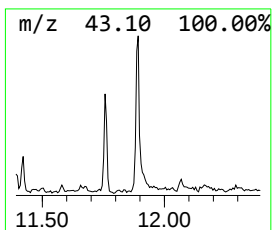
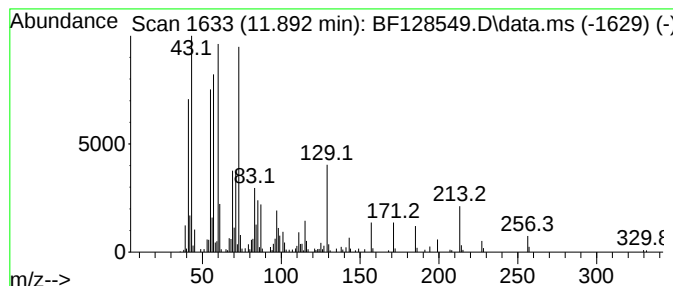
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.61 ng	229972	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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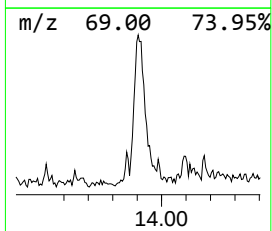
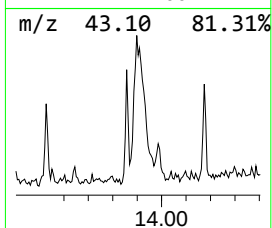
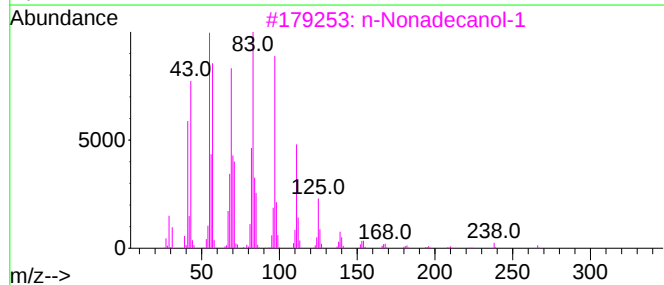
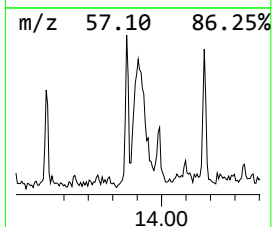
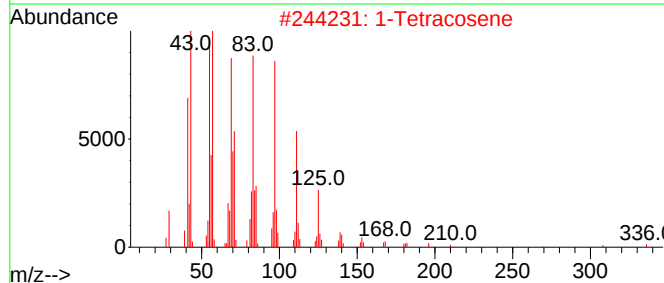
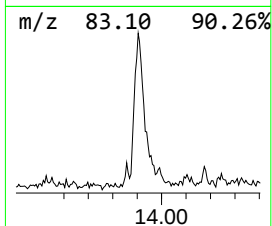
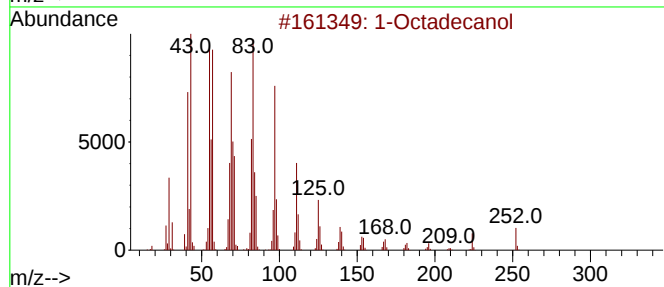
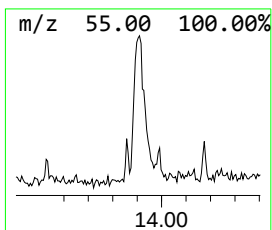
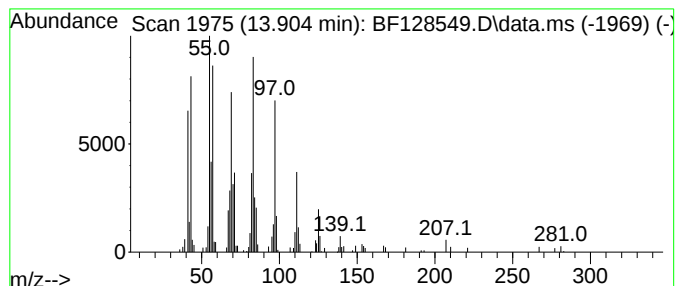
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Peak Number 4 1-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.97 ng	241488	Chrysene-d12	13.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecanol	270	C18H38O	000112-92-5	95
2		1-Tetracosene	336	C24H48	010192-32-2	94
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4		n-Heptadecanol-1	256	C17H36O	001454-85-9	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	90



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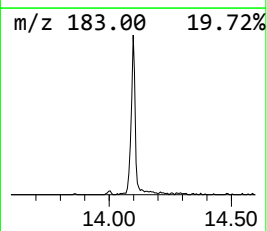
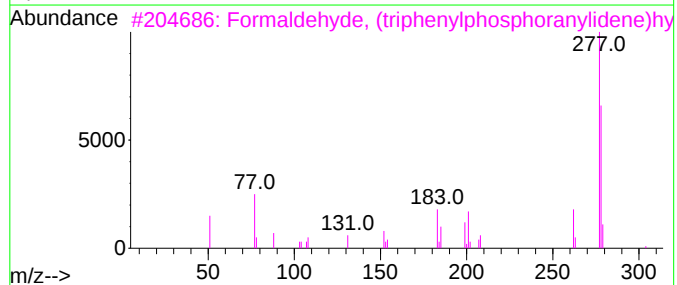
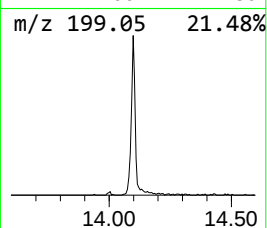
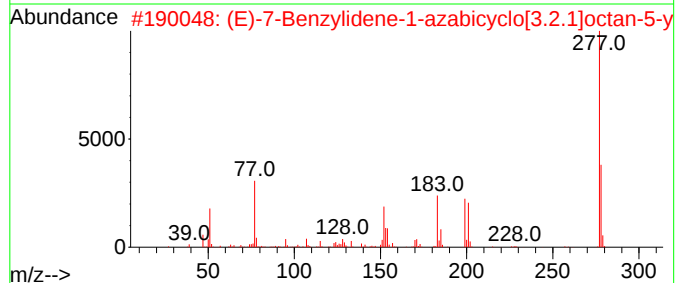
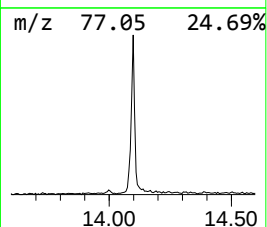
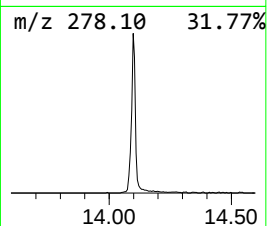
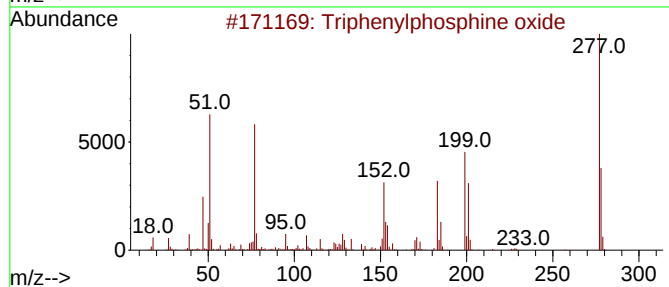
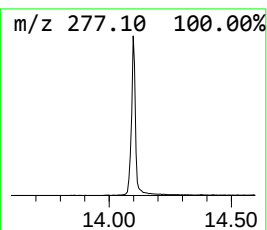
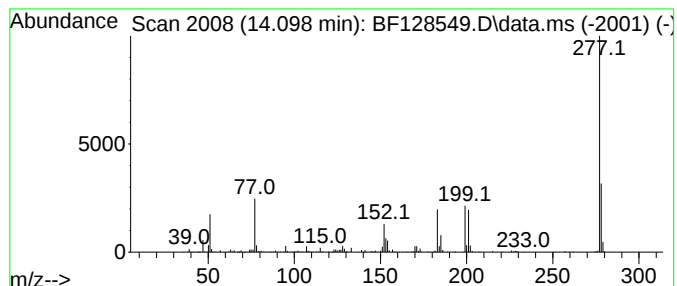
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	9.19 ng	558620	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32



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P023-SS001-1218-01

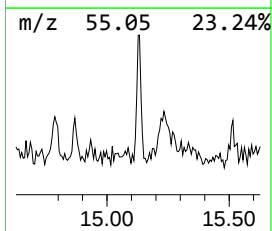
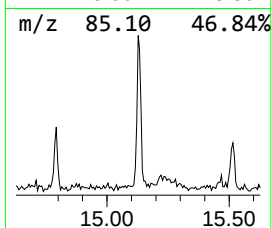
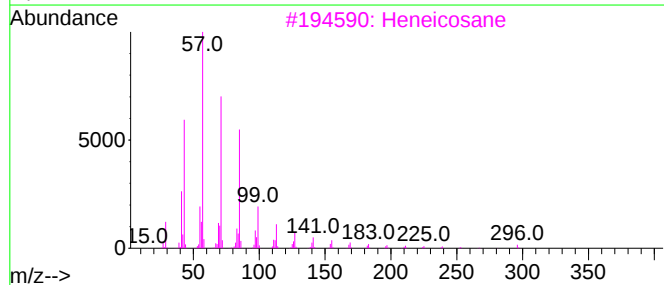
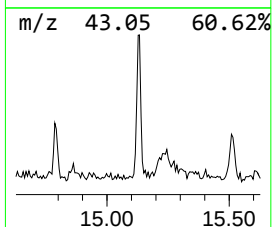
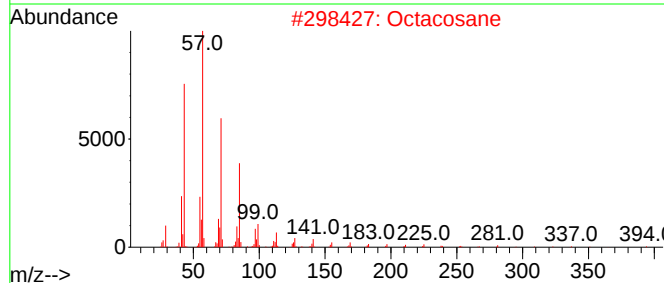
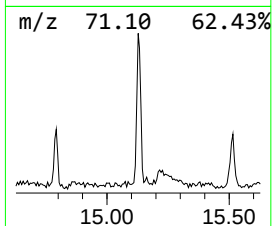
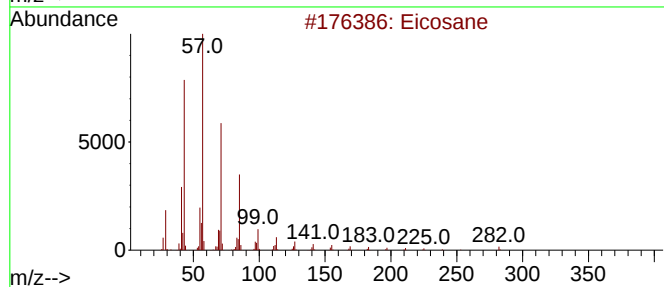
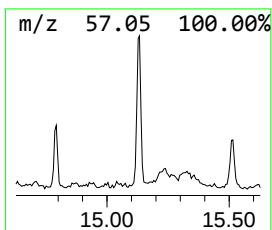
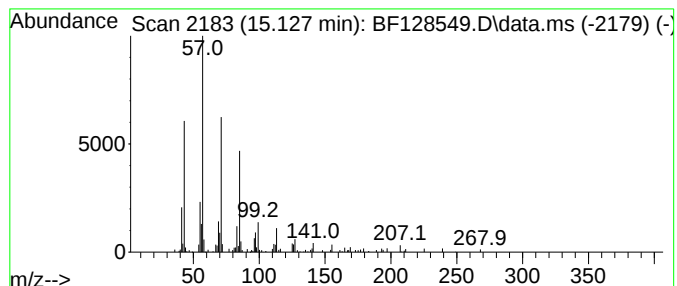
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.01 ng	99138	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128549.D
Acq On : 28 May 2022 15:35
Operator : CG\JU
Sample : N2933-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1218-01

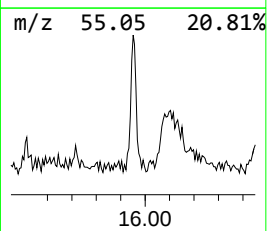
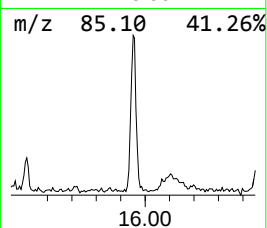
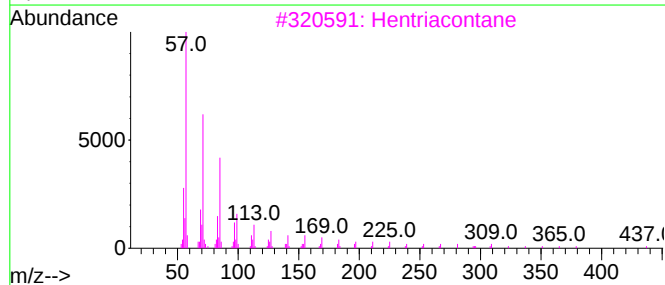
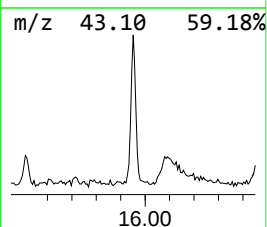
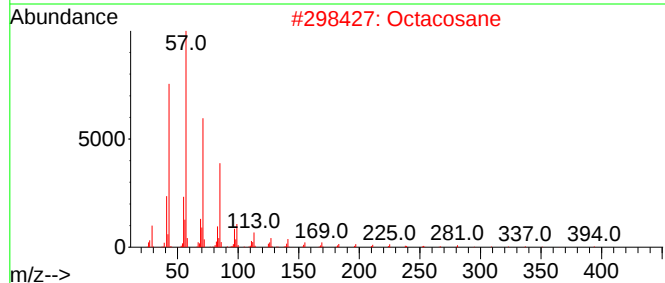
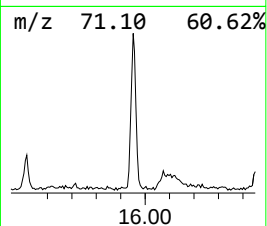
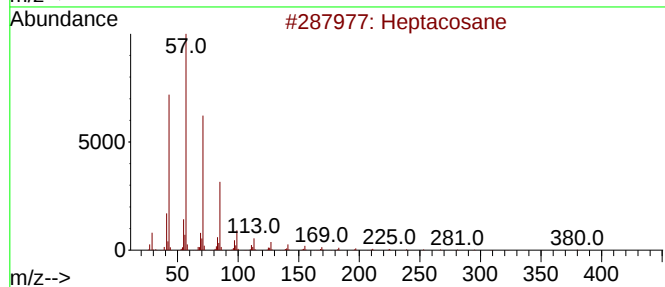
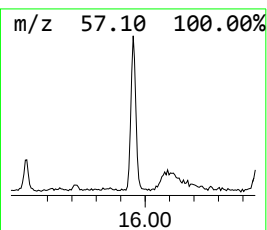
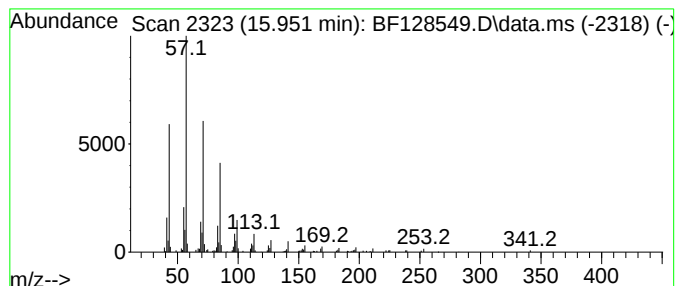
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	4.11 ng	202787	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128549.D
Acq On : 28 May 2022 15:35
Operator : CG\JU
Sample : N2933-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1218-01

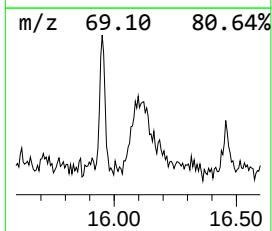
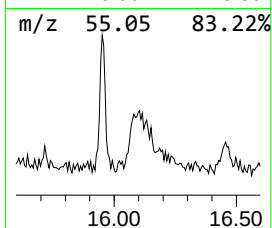
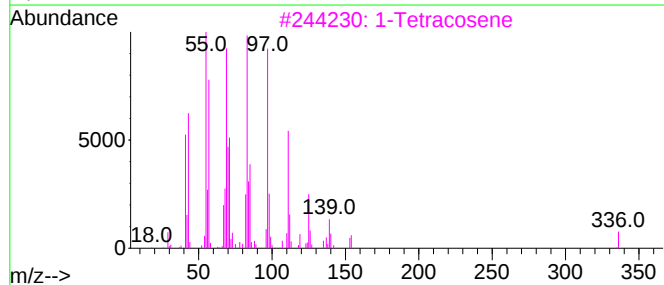
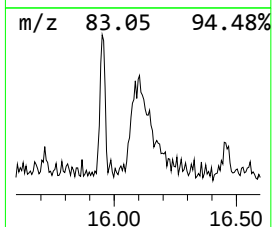
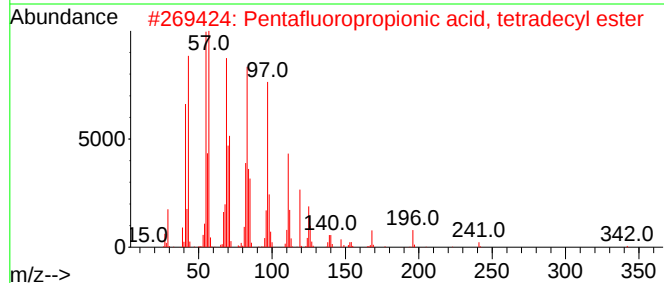
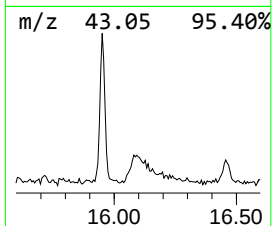
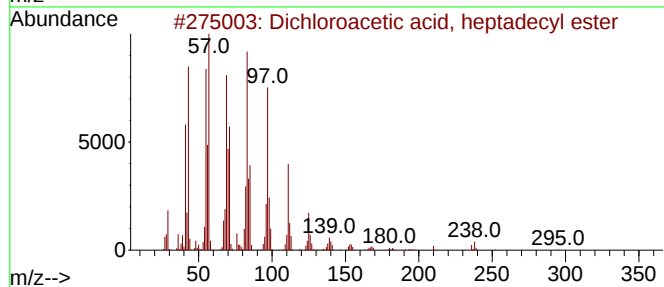
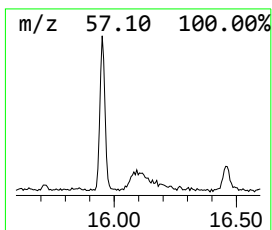
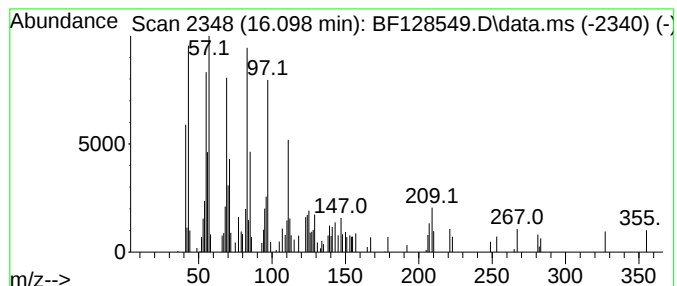
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	2.28 ng	112119	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	80
2			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	74
3			1-Tetracosene	336	C24H48	010192-32-2	72
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	68
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128549.D
Acq On : 28 May 2022 15:35
Operator : CG\JU
Sample : N2933-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1218-01

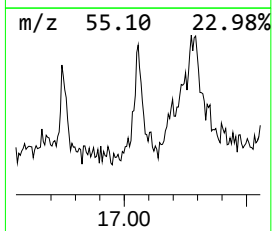
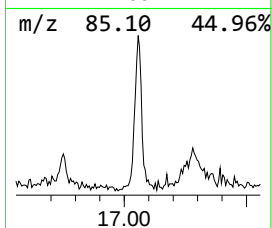
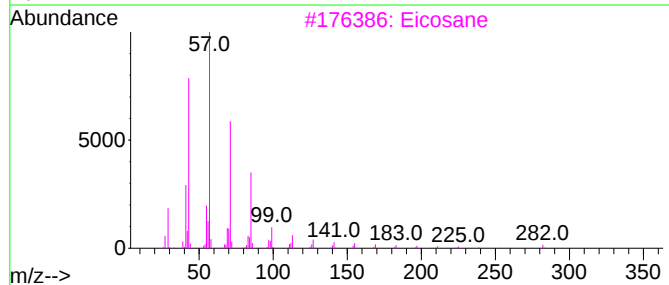
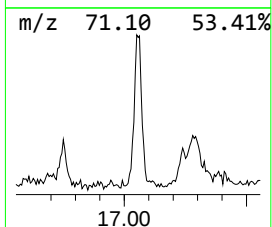
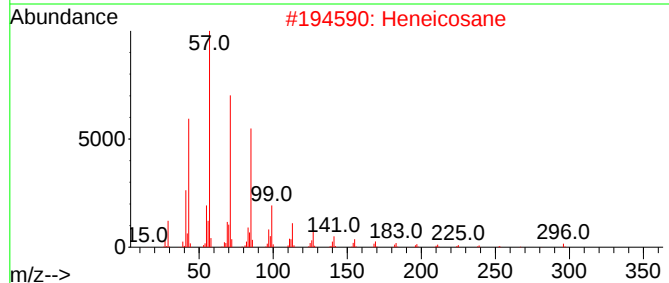
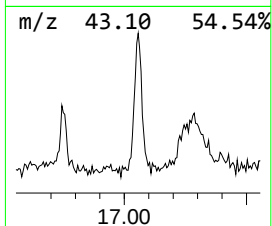
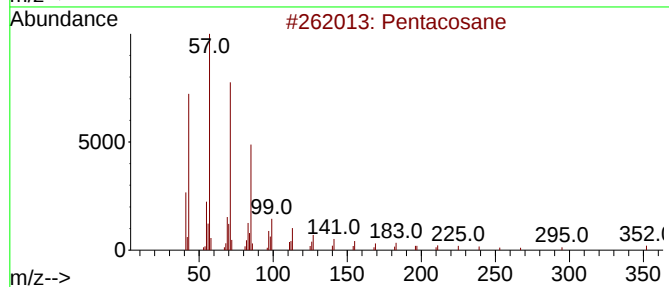
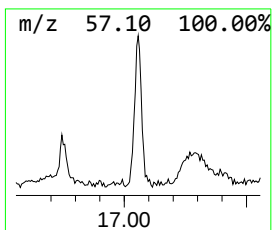
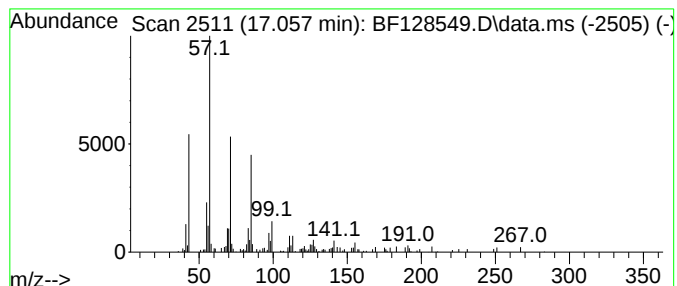
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	2.47 ng	121554	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Eicosane	282	C20H42	000112-95-8	91
4			Octadecane	254	C18H38	000593-45-3	91
5			Docosane	310	C22H46	000629-97-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128549.D
Acq On : 28 May 2022 15:35
Operator : CG\JU
Sample : N2933-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P023-SS001-1218-01

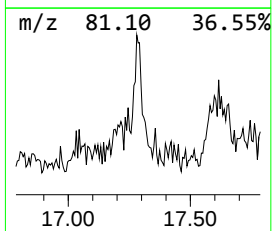
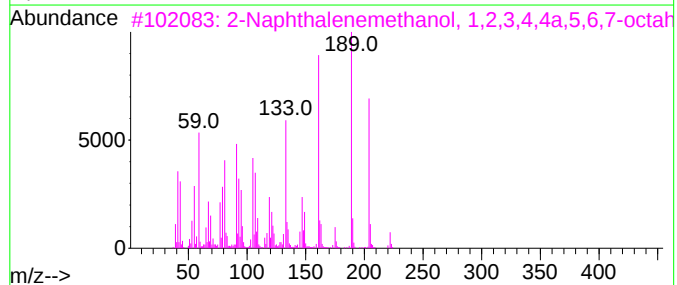
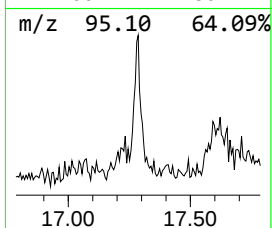
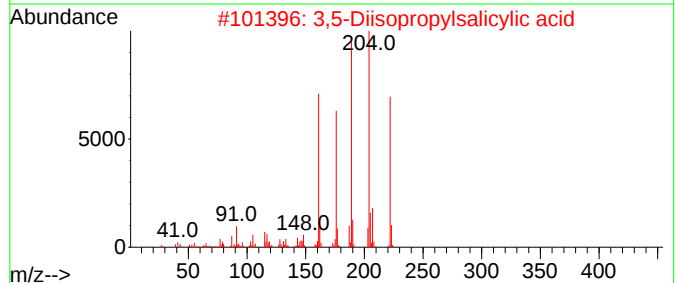
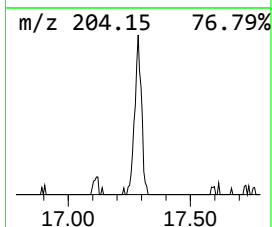
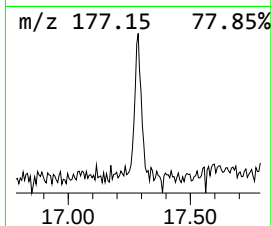
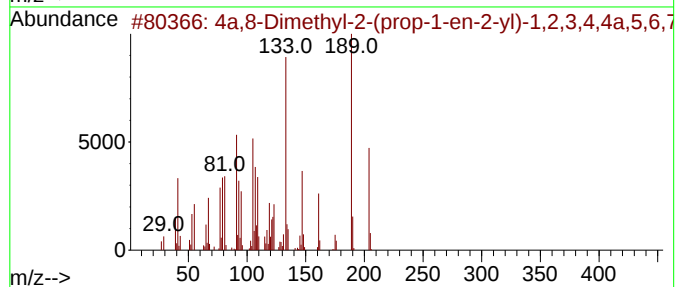
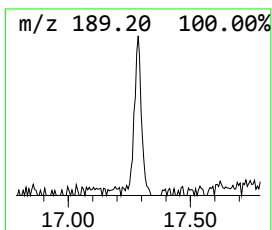
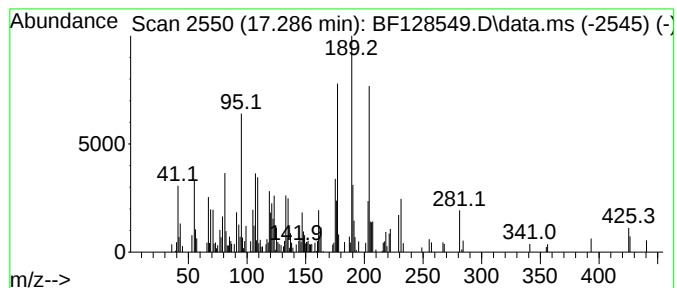
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 4a,8-Dimethyl-2-(prop-1-en-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	3.61 ng	177913	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	50
2			3,5-Diisopropylsalicylic acid	222	C13H18O3	002215-21-6	45
3			2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	45
4			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	43
5			Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128549.D
Acq On : 28 May 2022 15:35
Operator : CG\JU
Sample : N2933-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-1218-01

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
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Benzenesulfonam...	10.769	2.8	ng	245567	4	11.363	1761910	20.0
n-Hexadecanoic ...	11.892	2.6	ng	229972	4	11.363	1761910	20.0
1-Octadecanol	13.904	4.0	ng	241488	5	13.998	1216110	20.0
Triphenylphosph...	14.098	9.2	ng	558620	5	13.998	1216110	20.0
Eicosane	15.127	2.0	ng	99138	6	15.463	985627	20.0
Heptacosane	15.951	4.1	ng	202787	6	15.463	985627	20.0
Dichloroacetic ...	16.098	2.3	ng	112119	6	15.463	985627	20.0
Pentacosane	17.057	2.5	ng	121554	6	15.463	985627	20.0
4a,8-Dimethyl-2...	17.286	3.6	ng	177913	6	15.463	985627	20.0