

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128556.D
 Acq On : 28 May 2022 19:08
 Operator : CG\JU
 Sample : N2933-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P023-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: BF128556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.316	173	175	193	rBV	26134	63455	1.42%	0.201%
2	5.063	468	472	479	rVB	159171	190011	4.25%	0.601%
3	5.457	533	539	542	rBV	3496230	3831425	85.66%	12.120%
4	6.463	704	710	713	rBV	3496481	3877784	86.70%	12.267%
5	6.575	726	729	733	rBV	104891	80478	1.80%	0.255%
6	6.834	770	773	777	rBV	1049724	947632	21.19%	2.998%
7	7.398	864	869	872	rBV	2659153	2685038	60.03%	8.494%
8	8.116	987	991	995	rBV	1372513	1252177	28.00%	3.961%
9	9.198	1169	1175	1178	rBV	4974986	4472645	100.00%	14.149%
10	9.875	1286	1290	1293	rVB	1720031	1361792	30.45%	4.308%
11	10.663	1419	1424	1427	rBV	3052661	2722283	60.87%	8.612%
12	11.363	1539	1543	1546	rBV	1517731	1324769	29.62%	4.191%
13	11.757	1607	1610	1614	rVB	228716	190270	4.25%	0.602%
14	11.892	1629	1633	1647	rBV	550724	539591	12.06%	1.707%
15	12.469	1725	1731	1734	rBV	190622	173225	3.87%	0.548%
16	12.557	1742	1746	1748	rBV2	40101	51742	1.16%	0.164%
17	12.598	1751	1753	1763	rVV4	38315	67028	1.50%	0.212%
18	12.674	1763	1766	1774	rVV	129834	150649	3.37%	0.477%
19	12.951	1809	1813	1816	rBV	4011975	3606011	80.62%	11.407%
20	13.898	1968	1974	1986	rVB4	185969	537572	12.02%	1.701%
21	13.998	1987	1991	1995	rBV	1021874	929839	20.79%	2.941%
22	14.098	2001	2008	2015	rBV	494177	549254	12.28%	1.737%
23	14.404	2051	2060	2061	rBV8	35964	88066	1.97%	0.279%
24	14.527	2078	2081	2093	rVB7	55184	103072	2.30%	0.326%
25	15.133	2180	2184	2188	rVB	57255	64433	1.44%	0.204%
26	15.468	2235	2241	2246	rBV	680555	882874	19.74%	2.793%
27	15.951	2319	2323	2331	rVB	63650	92893	2.08%	0.294%
28	16.104	2339	2349	2359	rBV7	49356	218617	4.89%	0.692%
29	16.751	2456	2459	2468	rVB8	28382	56794	1.27%	0.180%
30	17.056	2503	2511	2516	rBV4	36227	90525	2.02%	0.286%
31	17.286	2545	2550	2564	rVB8	87157	230308	5.15%	0.729%
32	17.609	2596	2605	2617	rBV8	40617	179683	4.02%	0.568%

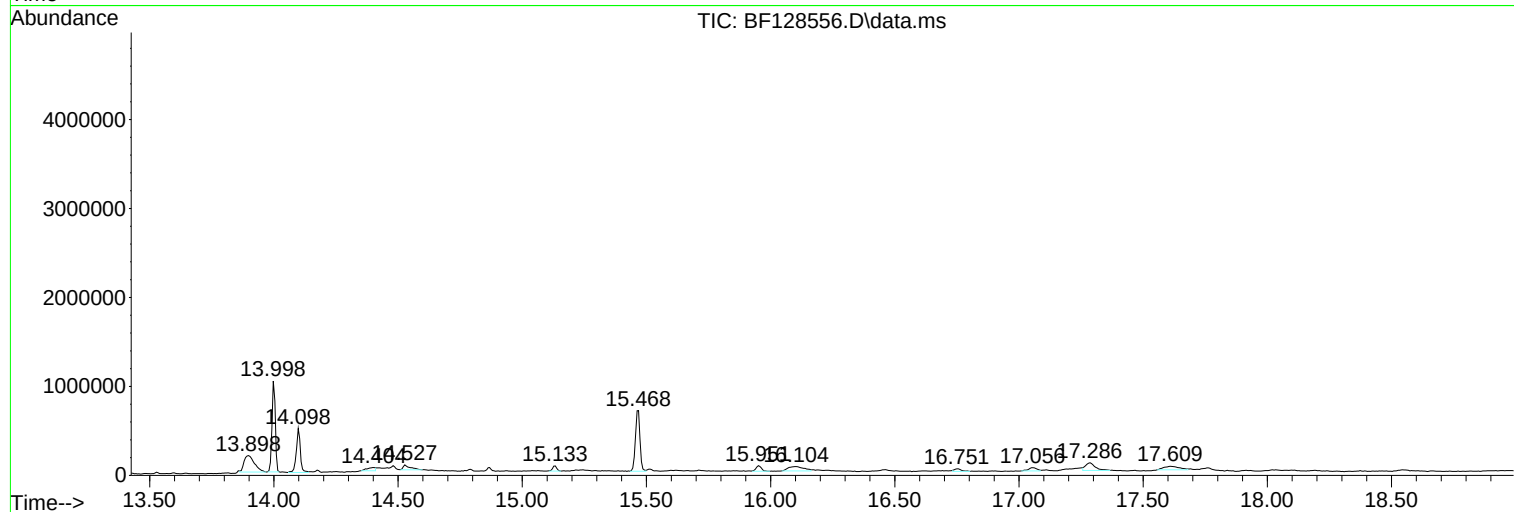
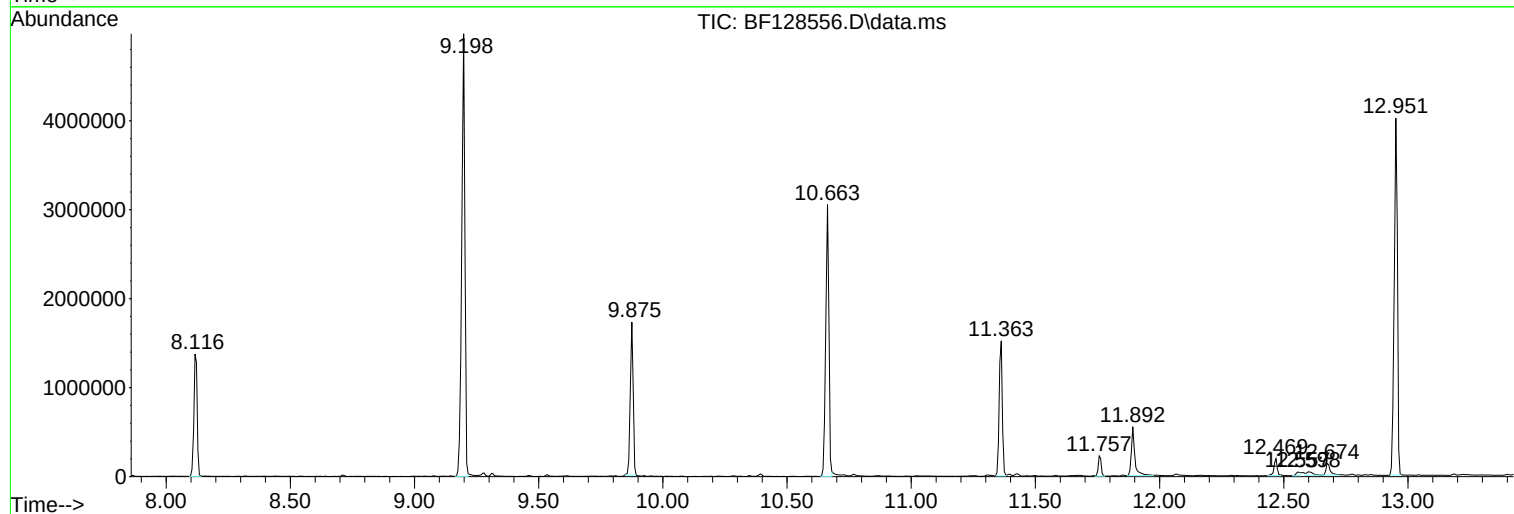
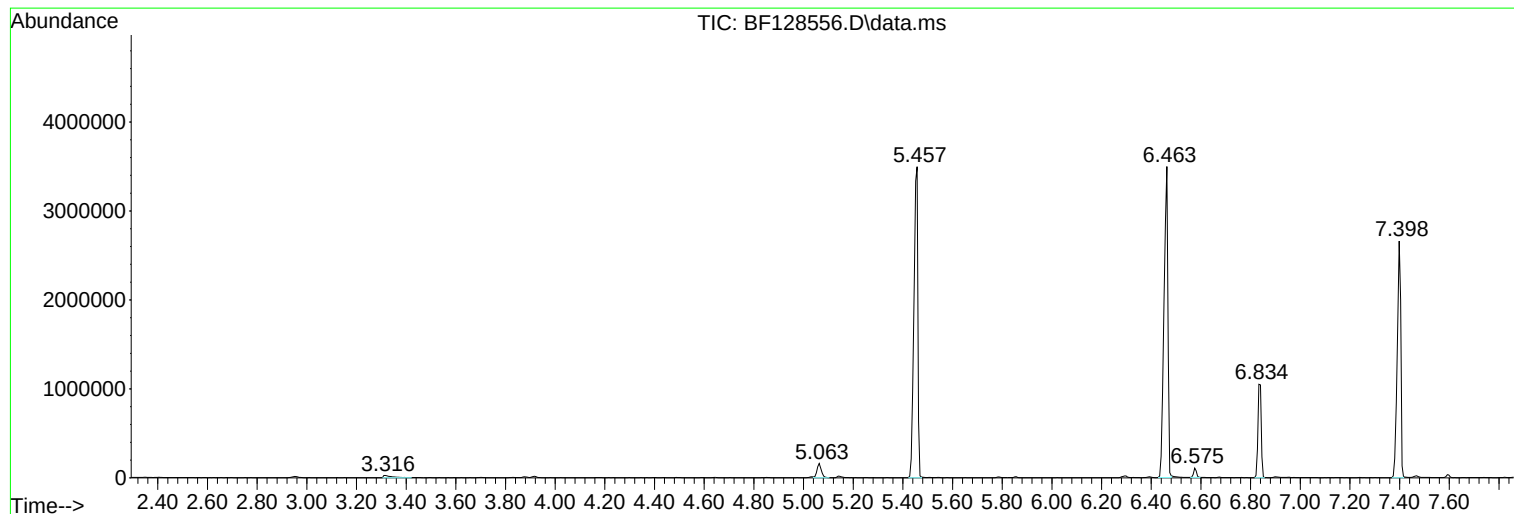
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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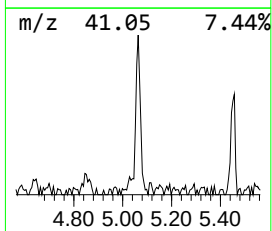
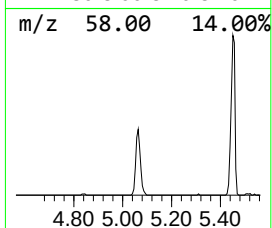
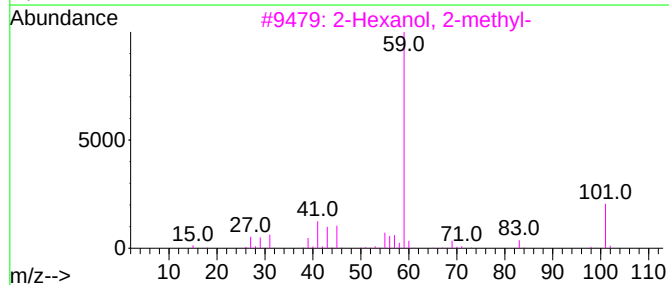
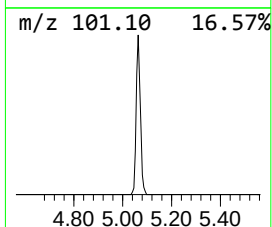
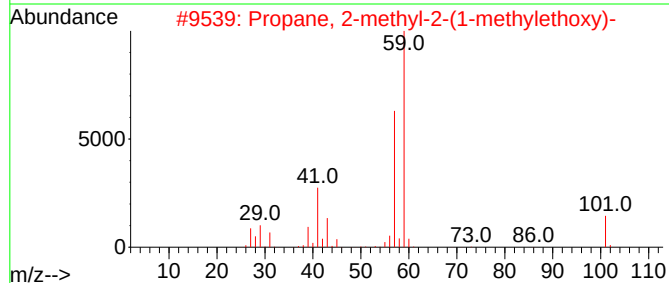
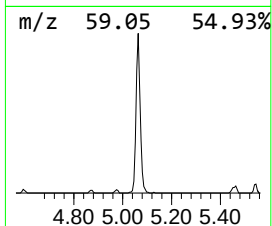
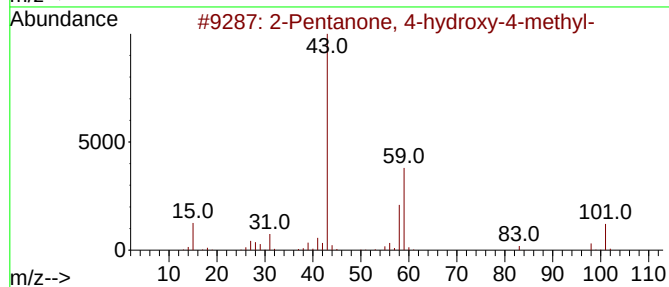
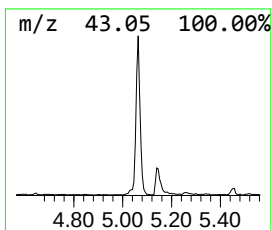
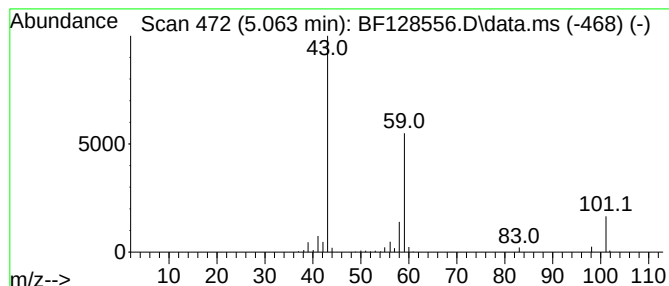
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	4.01 ng	190011	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	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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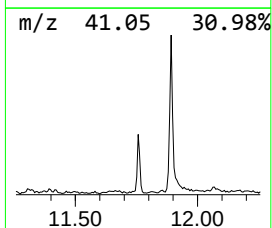
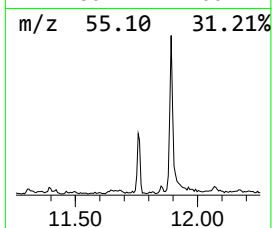
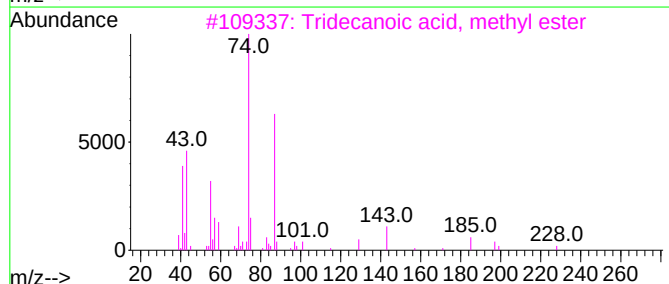
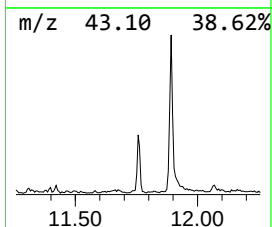
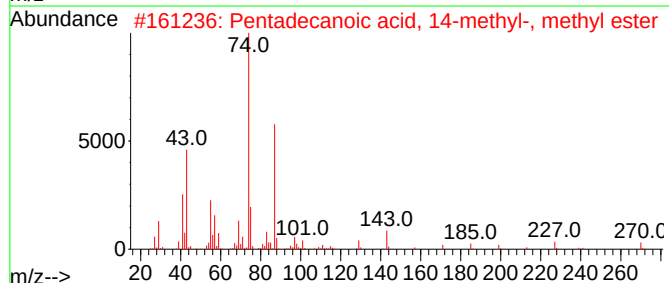
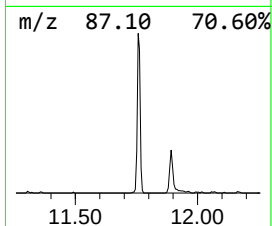
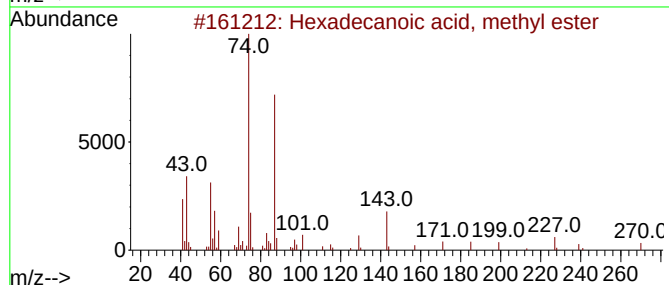
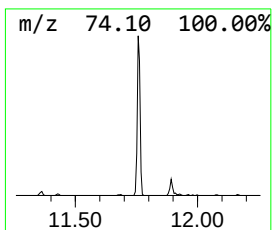
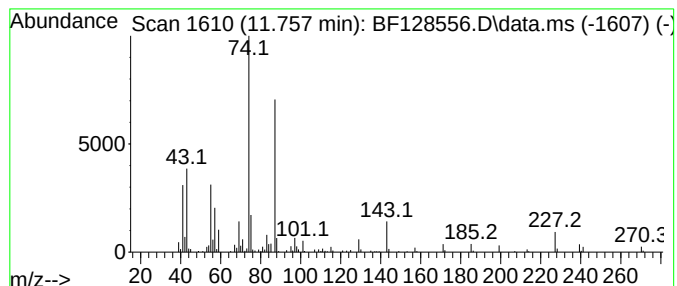
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.757	2.87 ng	190270	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	83



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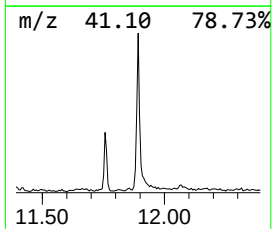
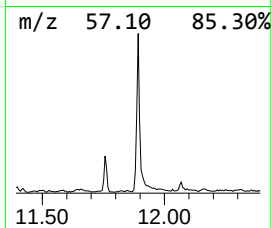
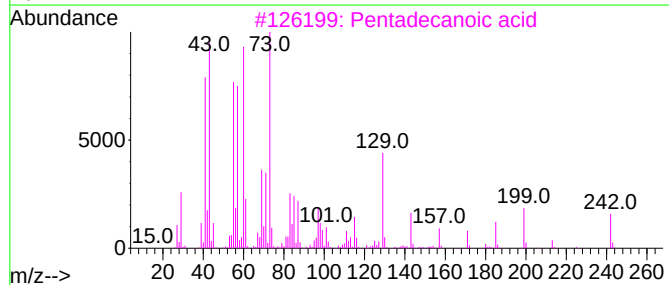
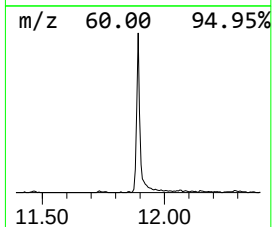
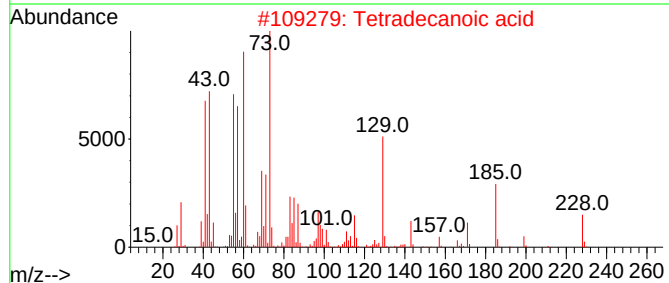
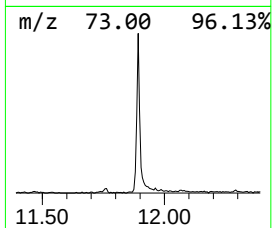
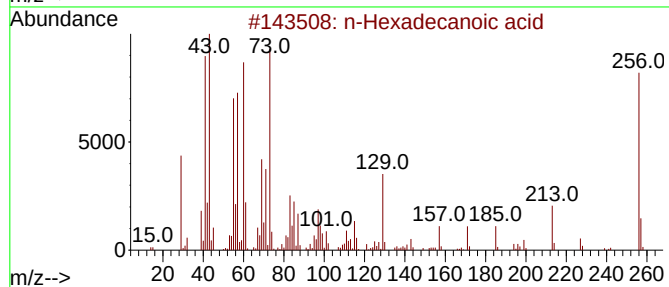
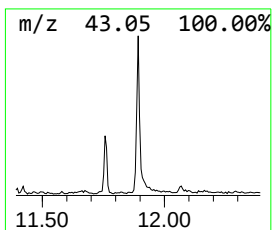
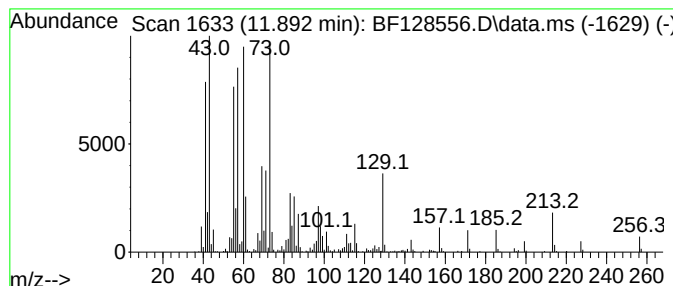
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	8.15 ng	539591	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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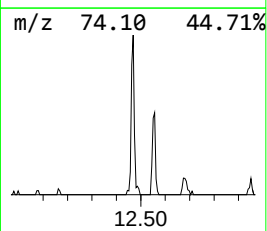
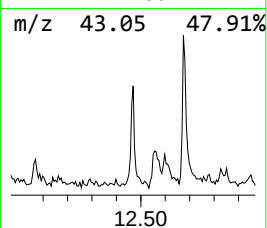
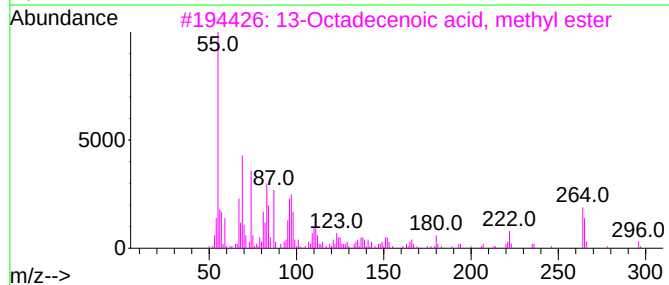
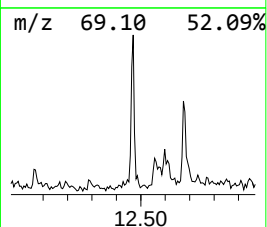
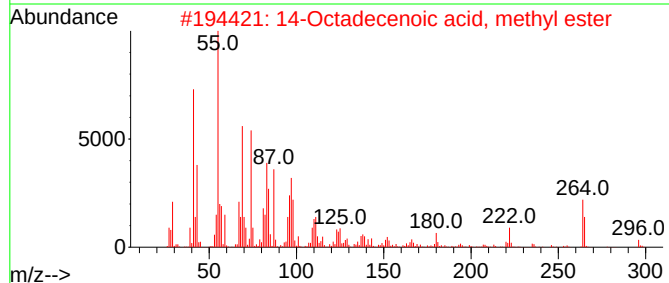
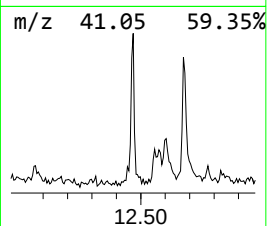
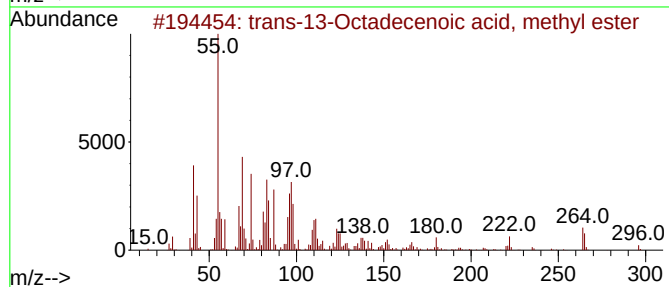
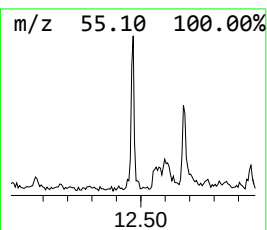
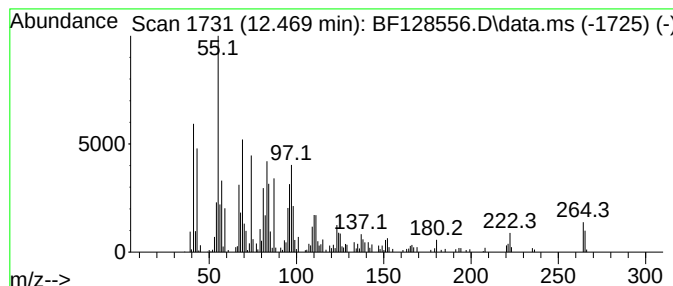
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Peak Number 4 trans-13-Octadecenoic acid,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	2.62 ng	173225	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
2			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
5			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	76



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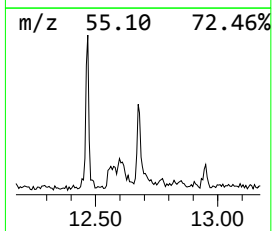
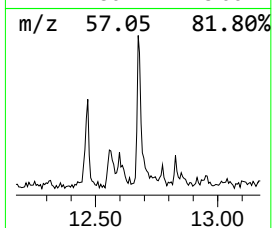
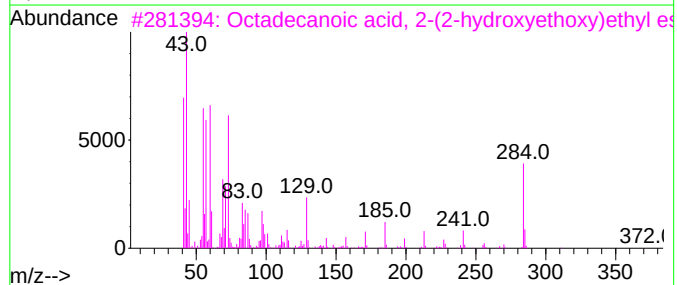
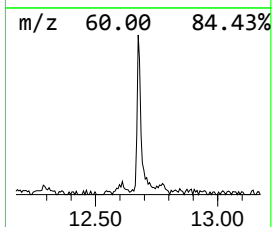
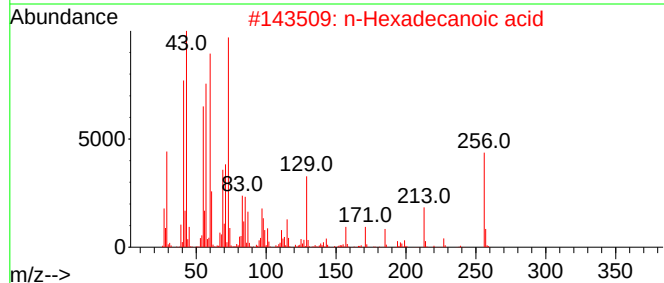
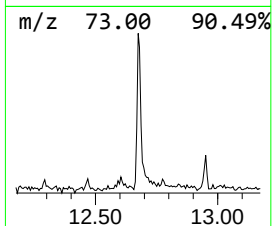
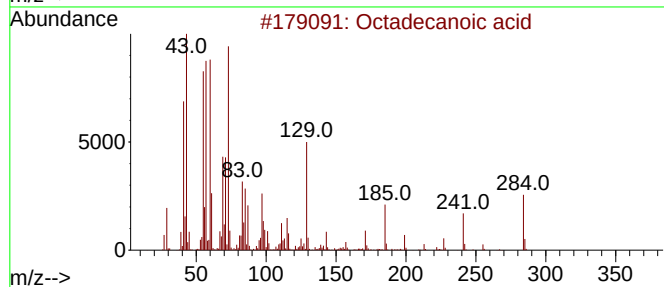
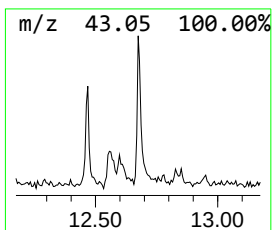
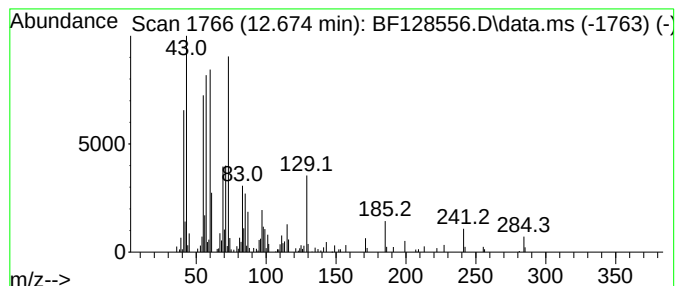
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Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	2.27 ng	150649	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	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	52



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P023-SS001-0612-01

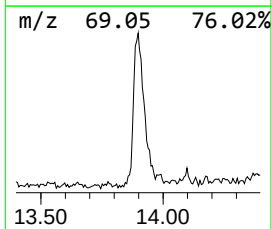
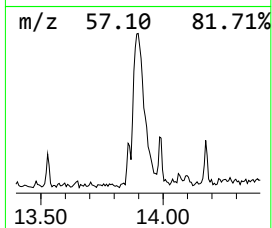
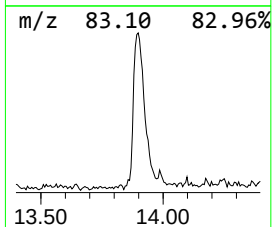
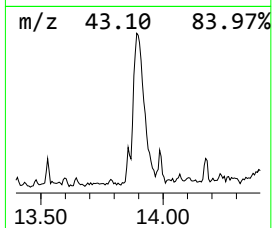
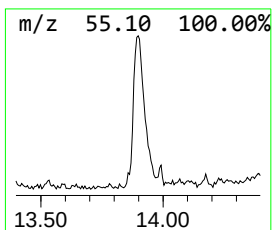
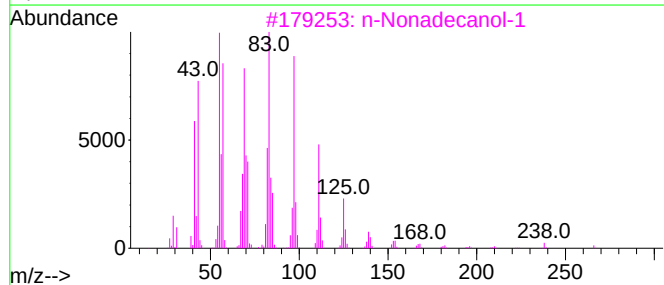
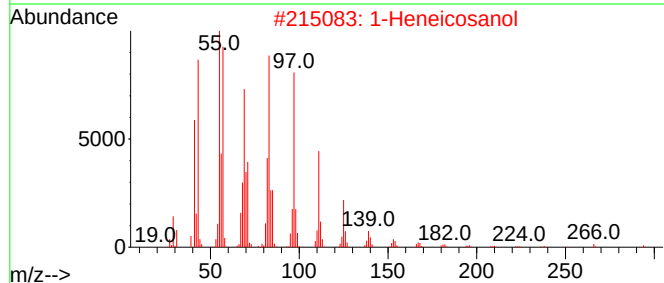
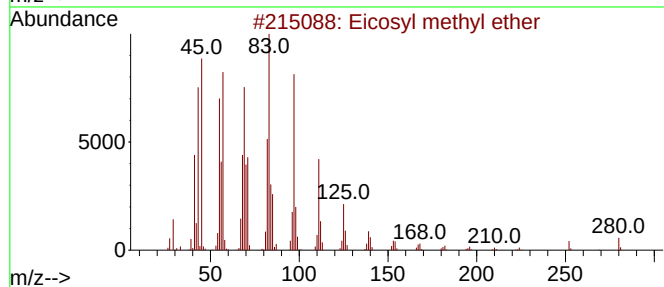
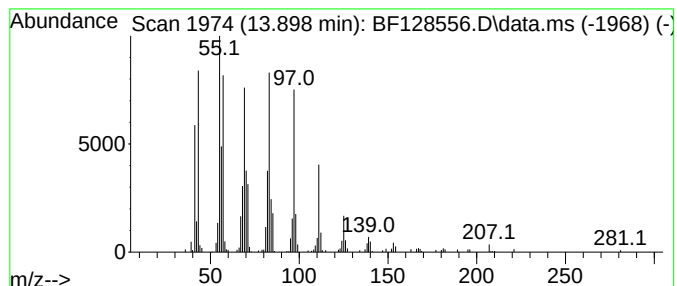
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosyl methyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	11.56 ng	537572	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl methyl ether	312	C21H44O	1000406-29-4	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5			1-Octadecanol	270	C18H38O	000112-92-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
Sample : N2933-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-0612-01

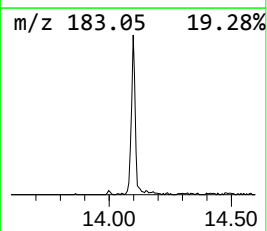
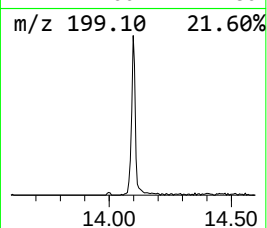
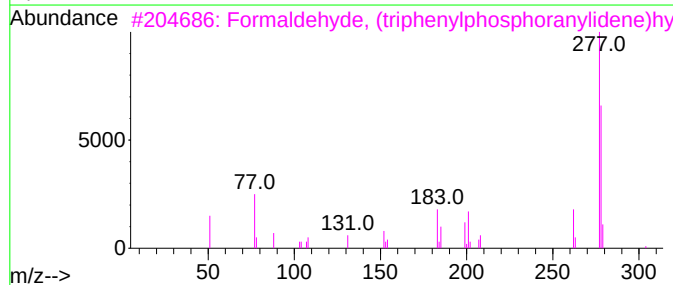
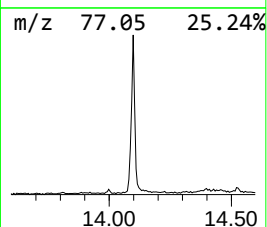
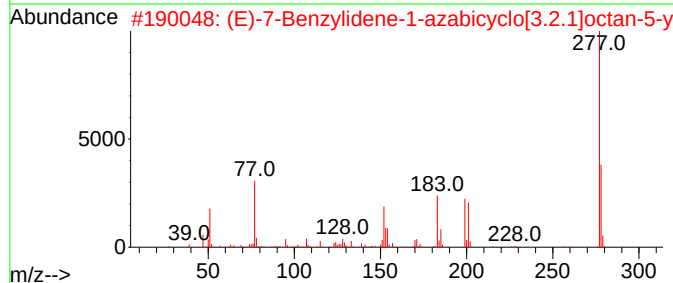
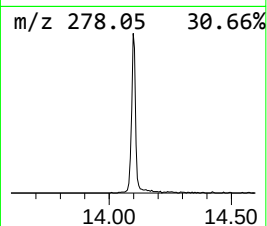
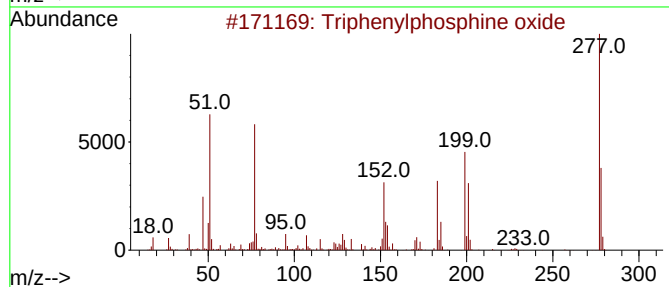
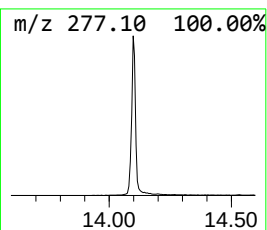
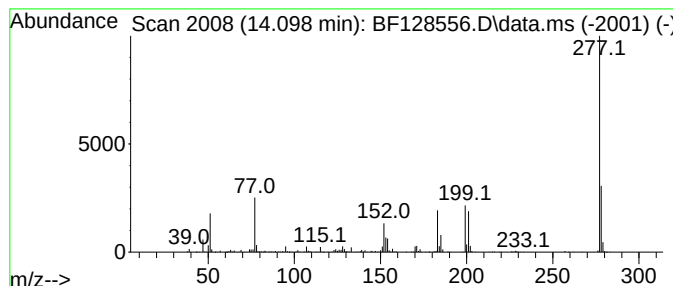
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	11.81 ng	549254	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	95
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
Sample : N2933-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P023-SS001-0612-01

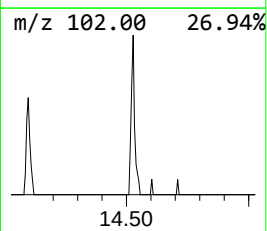
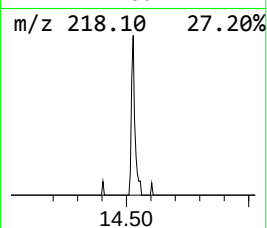
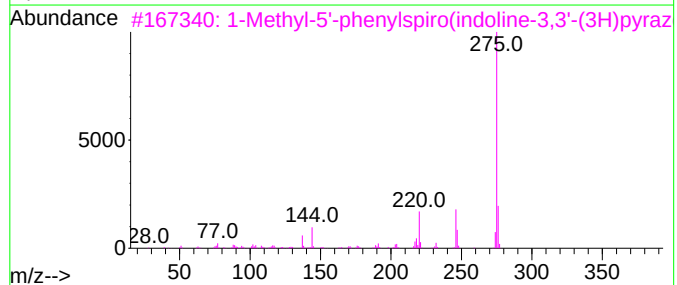
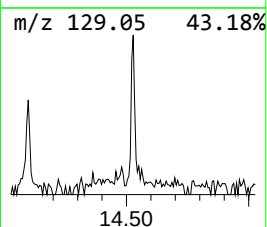
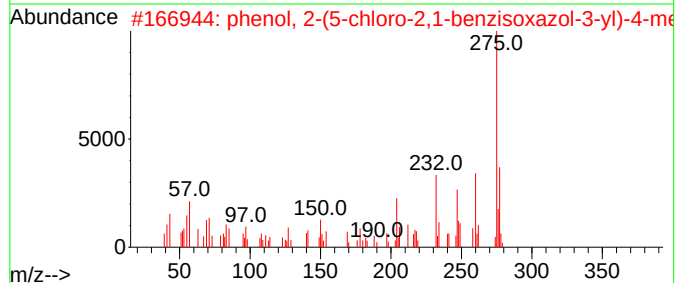
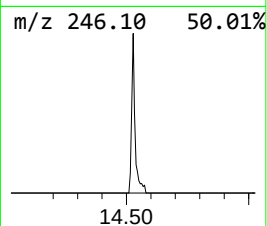
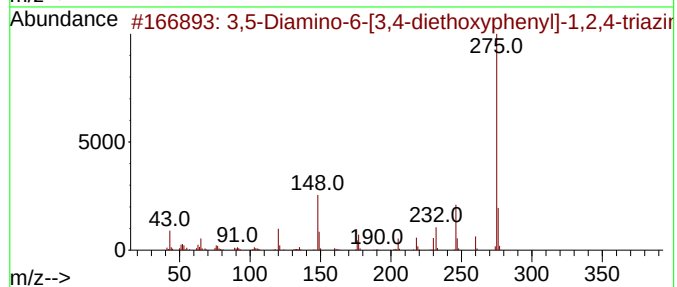
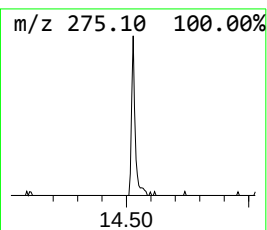
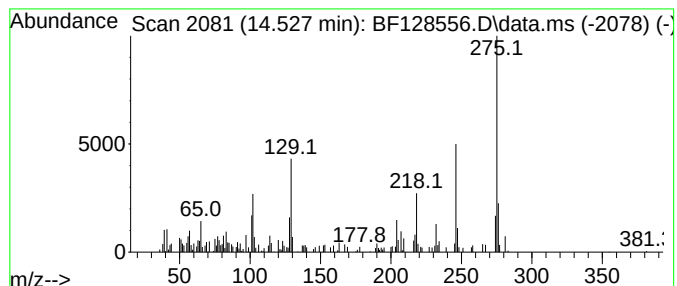
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.527 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	2.22 ng	103072	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Diamino-6-[3,4-diethoxypheny...	275	C13H17N5O2	058848-69-4	46
2			phenol, 2-(5-chloro-2,1-benzisox...	275	C14H10ClNO3	1000397-06-6	45
3			1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	43
4			Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	43
5			Ethyl 2-cyano-2-(9-fluorenyliden...	275	C18H13NO2	014003-25-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
Sample : N2933-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P023-SS001-0612-01

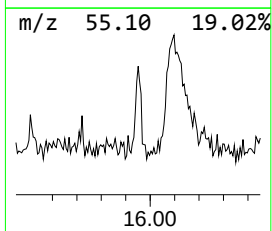
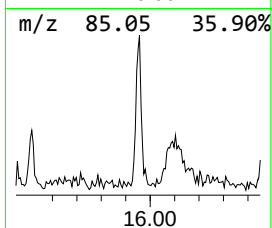
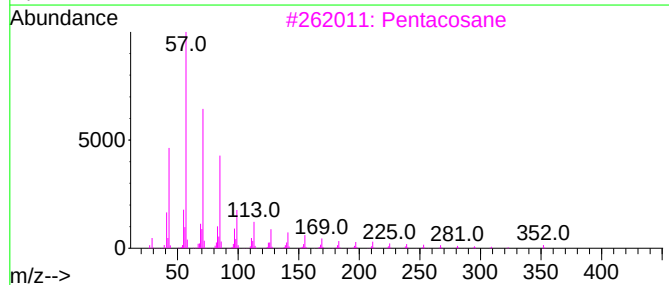
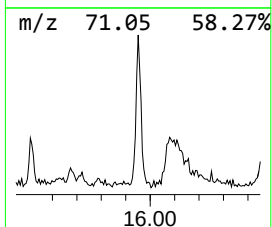
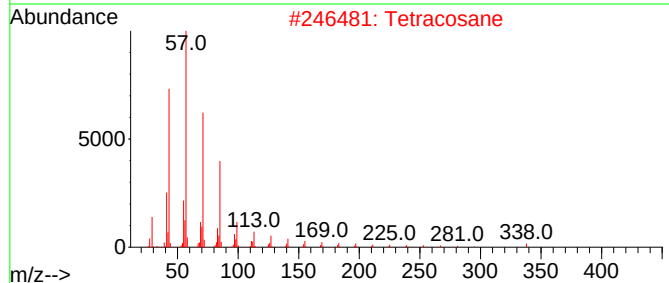
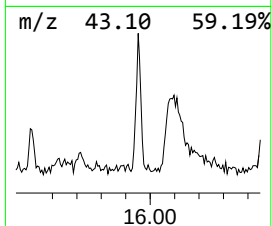
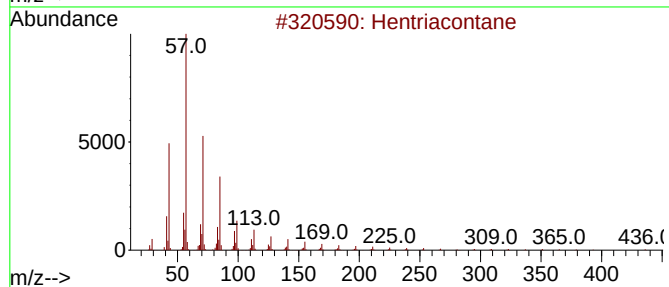
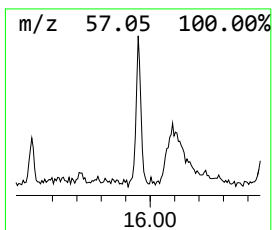
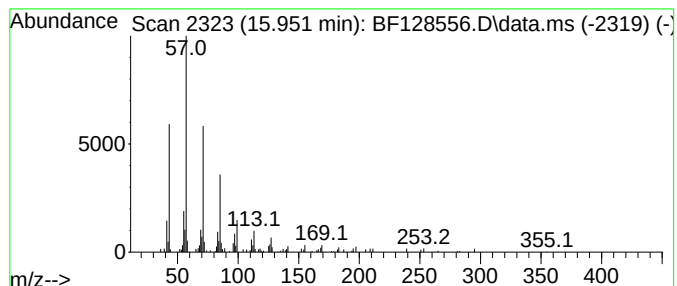
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.10 ng	92893	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			Pentacosane	352	C25H52	000629-99-2	87
4			Octacosane	394	C28H58	000630-02-4	87
5			triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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P023-SS001-0612-01

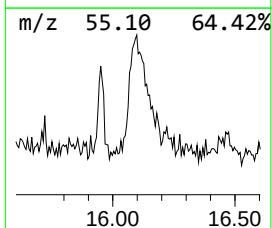
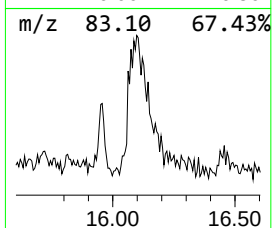
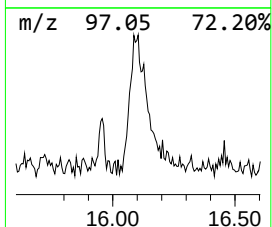
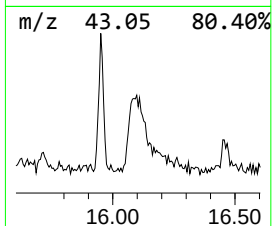
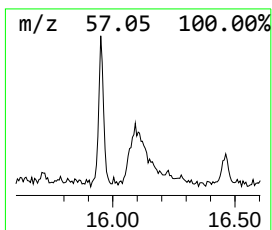
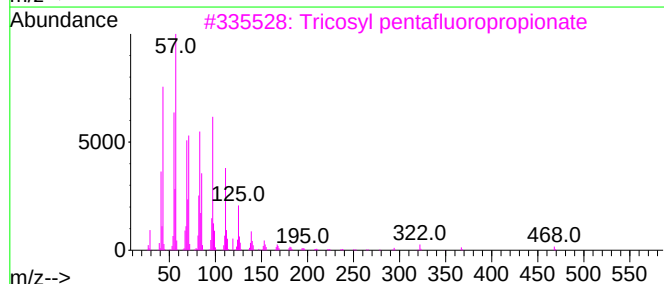
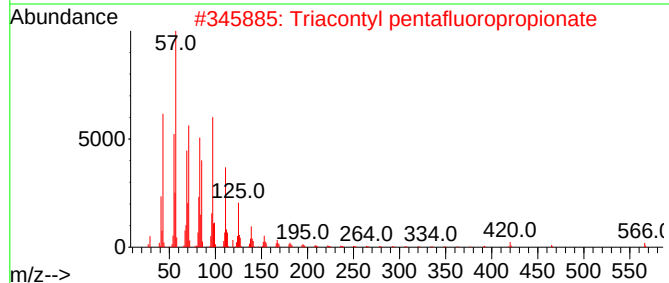
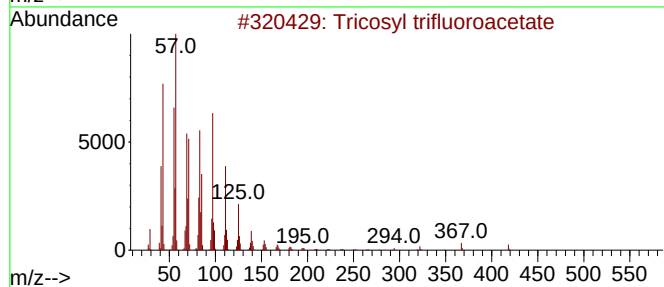
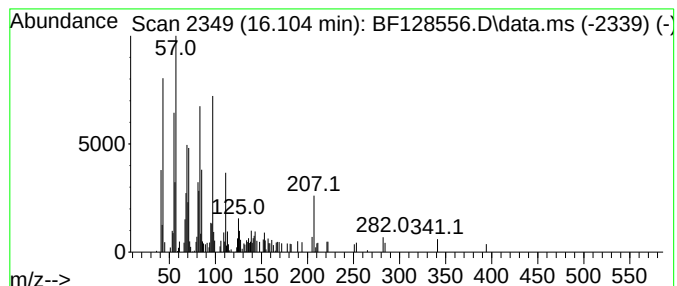
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	4.95 ng	218617	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	81
2			Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	74
3			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	74
4			Carbonic acid, but-2-yn-1-yl eic...	394	C25H46O3	1000383-21-4	74
5			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
Sample : N2933-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P023-SS001-0612-01

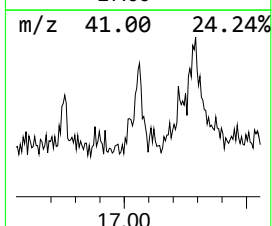
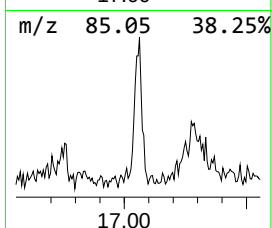
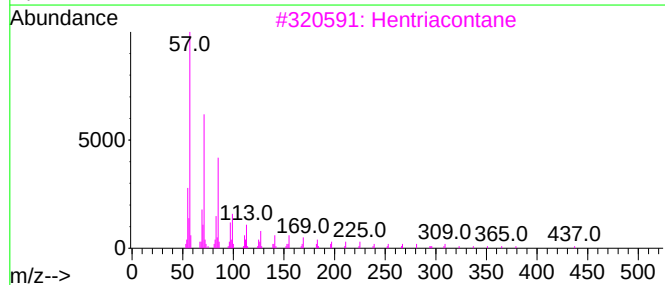
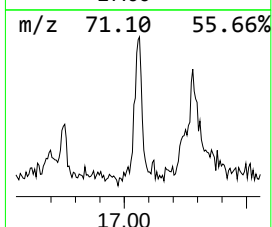
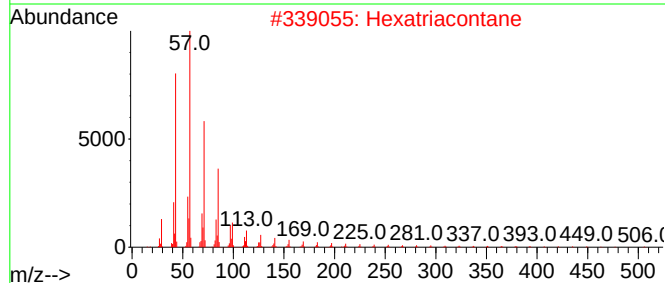
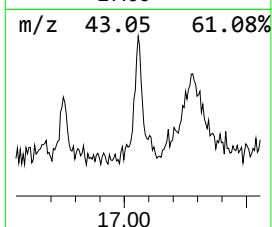
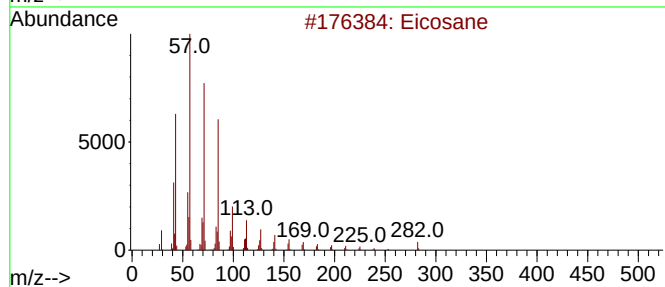
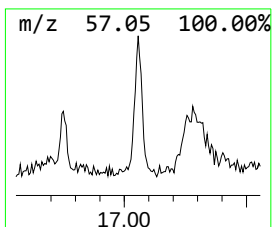
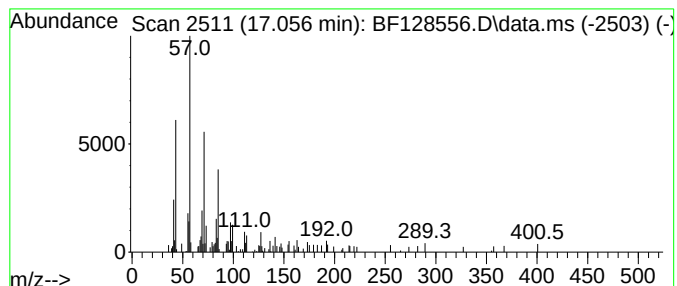
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.056	2.05 ng	90525	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	89
2			Hexatriacontane	507	C36H74	000630-06-8	74
3			Hentriacontane	437	C31H64	000630-04-6	74
4			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	74
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P023-SS001-0612-01

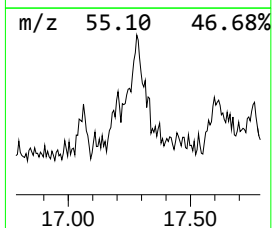
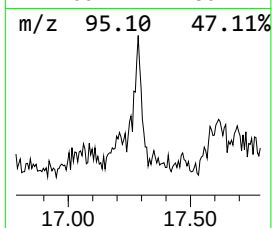
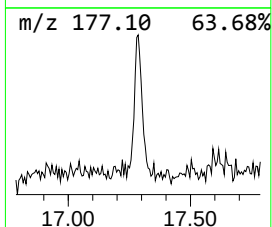
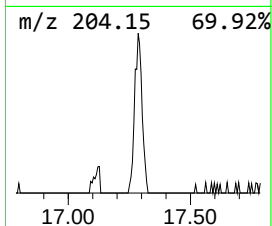
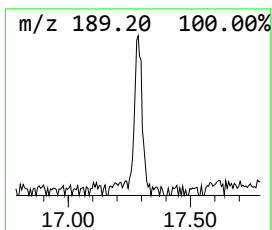
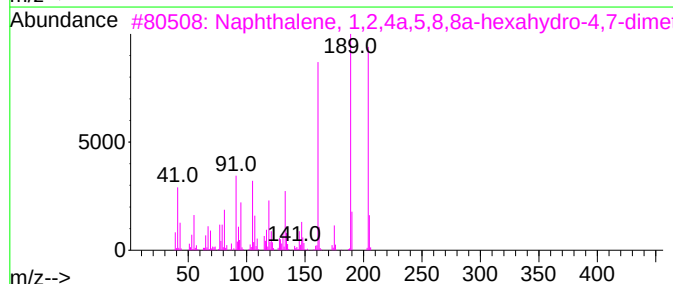
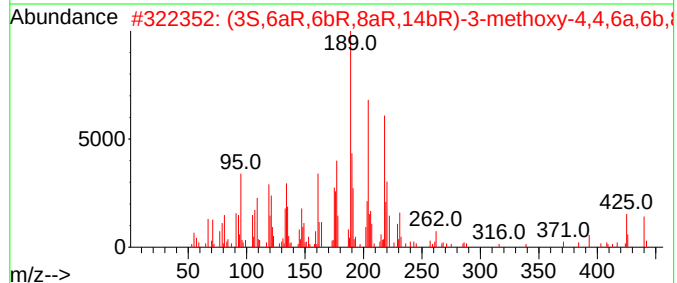
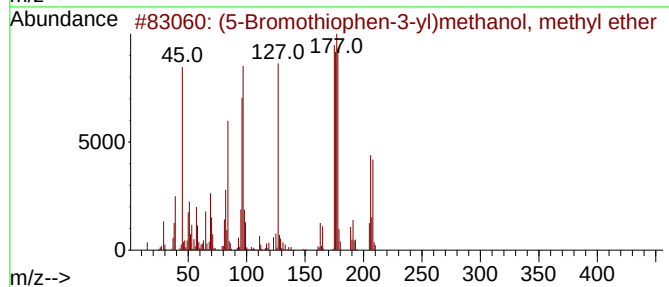
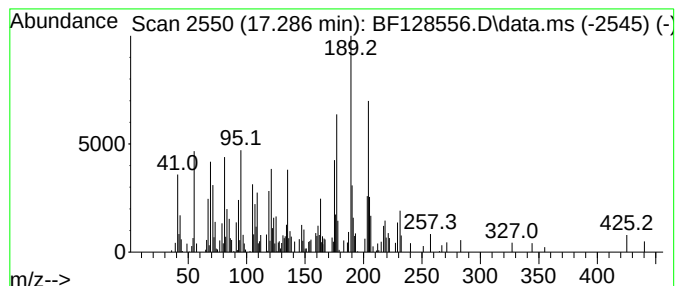
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 (5-Bromothiophen-3-yl)metha... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	5.22 ng	230308	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(5-Bromothiophen-3-yl)methanol, ...	206	C6H7BrOS	1000505-64-0	56
2		(3S,6aR,6bR,8aR,14bR)-3-methoxy-...	440	C31H52O	1000441-97-8	52
3		Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	38
4		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	35
5		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
Sample : N2933-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS001-0612-01

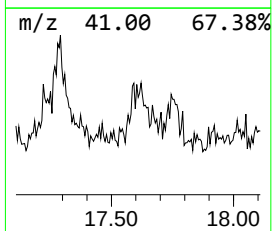
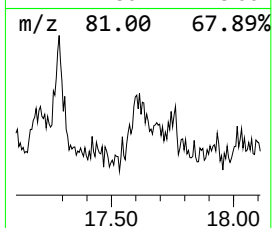
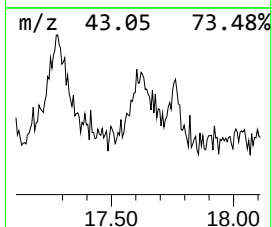
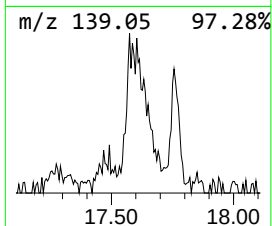
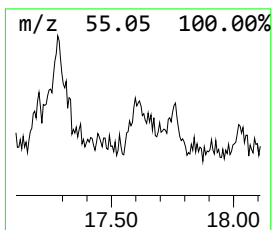
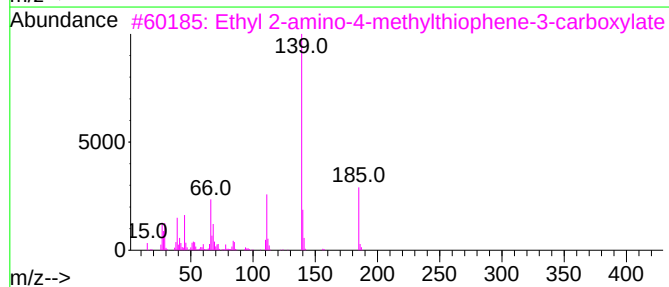
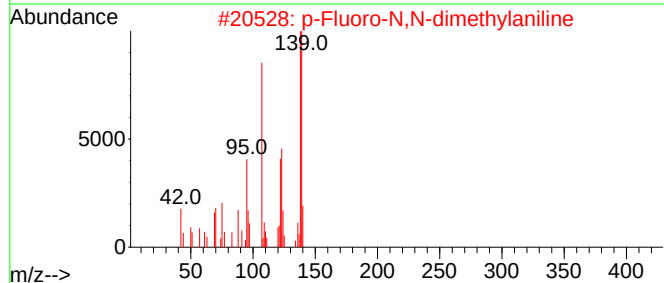
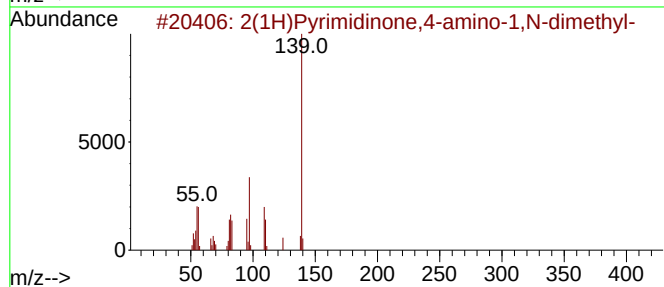
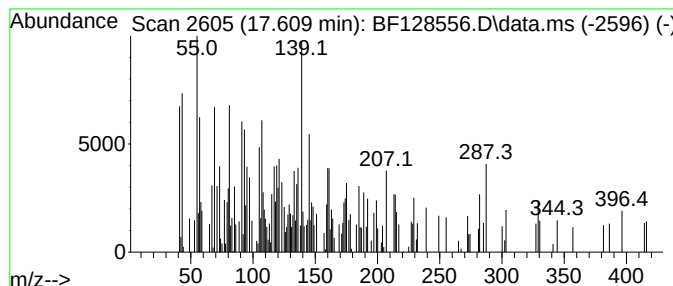
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.609 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.609	4.07 ng	179683	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)Pyrimidinone,4-amino-1,N-di...	139	C6H9N3O	006220-49-1	18		
2	p-Fluoro-N,N-dimethylaniline	139	C8H10FN	000403-46-3	18		
3	Ethyl 2-amino-4-methylthiophene-...	185	C8H11NO2S	043088-42-2	14		
4	3-Chlorobenzoic acid, [1-(3-amin...	287	C15H14ClN3O	1000303-03-5	14		
5	(R)-Noradrenaline	169	C8H11NO3	000149-95-1	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128556.D
Acq On : 28 May 2022 19:08
Operator : CG\JU
Sample : N2933-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-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-...	5.063	4.0	ng	190011	1	6.839	947632	20.0
Hexadecanoic ac...	11.757	2.9	ng	190270	4	11.363	1324770	20.0
n-Hexadecanoic ...	11.892	8.2	ng	539591	4	11.363	1324770	20.0
trans-13-Octade...	12.469	2.6	ng	173225	4	11.363	1324770	20.0
Octadecanoic acid	12.674	2.3	ng	150649	4	11.363	1324770	20.0
Eicosyl methyl ...	13.898	11.6	ng	537572	5	13.998	929839	20.0
Triphenylphosph...	14.098	11.8	ng	549254	5	13.998	929839	20.0
unknown14.527	14.527	2.2	ng	103072	5	13.998	929839	20.0
Hentriacontane	15.951	2.1	ng	92893	6	15.468	882874	20.0
Tricosyl triflu...	16.104	5.0	ng	218617	6	15.468	882874	20.0
Eicosane	17.056	2.0	ng	90525	6	15.468	882874	20.0
(5-Bromothiophe...	17.286	5.2	ng	230308	6	15.468	882874	20.0
unknown17.609	17.609	4.1	ng	179683	6	15.468	882874	20.0