

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128555.D
 Acq On : 28 May 2022 18:38
 Operator : CG\JU
 Sample : N2933-18
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P023-SS004-0006-01

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: BF128555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.322	173	176	192	rBV	32234	65733	1.41%	0.205%
2	5.069	470	473	481	rVB	53461	65438	1.41%	0.204%
3	5.457	533	539	542	rBV	3840733	3862684	83.11%	12.053%
4	6.463	704	710	713	rBV	3714025	3947410	84.93%	12.318%
5	6.575	726	729	734	rVB	94166	69043	1.49%	0.215%
6	6.834	770	773	777	rVB	1075520	979653	21.08%	3.057%
7	7.398	864	869	872	rBV	2765181	2734852	58.84%	8.534%
8	7.592	897	902	907	rVB	50748	49733	1.07%	0.155%
9	8.116	987	991	995	rBV	1436659	1269918	27.32%	3.963%
10	9.198	1169	1175	1178	rBV	5195357	4647748	100.00%	14.503%
11	9.822	1275	1281	1285	rBV	121125	96090	2.07%	0.300%
12	9.875	1285	1290	1293	rBV	1743388	1408581	30.31%	4.395%
13	10.663	1419	1424	1427	rBV	3114794	2800128	60.25%	8.738%
14	10.769	1438	1442	1452	rVB	318753	266634	5.74%	0.832%
15	11.363	1539	1543	1546	rBV	1595324	1344059	28.92%	4.194%
16	11.757	1607	1610	1614	rVB	197900	165217	3.55%	0.516%
17	11.892	1629	1633	1637	rBV	341943	317789	6.84%	0.992%
18	12.469	1724	1731	1734	rBV	211204	189628	4.08%	0.592%
19	12.674	1763	1766	1780	rBV	93098	110453	2.38%	0.345%
20	12.951	1809	1813	1816	rBV	4067492	3772784	81.17%	11.773%
21	13.910	1970	1976	1986	rVB3	93550	251379	5.41%	0.784%
22	13.998	1986	1991	1995	rBV2	1054243	1090529	23.46%	3.403%
23	14.098	2000	2008	2013	rBV	490703	555401	11.95%	1.733%
24	15.133	2180	2184	2189	rVB	65752	82358	1.77%	0.257%
25	15.468	2235	2241	2246	rBV	668816	896482	19.29%	2.797%
26	15.951	2319	2323	2330	rVB	76909	111183	2.39%	0.347%
27	16.104	2341	2349	2361	rBV	45524	184683	3.97%	0.576%
28	16.751	2455	2459	2467	rVB6	44853	84151	1.81%	0.263%
29	17.057	2504	2511	2519	rBV3	58676	134399	2.89%	0.419%
30	17.286	2544	2550	2562	rVB2	217240	492717	10.60%	1.537%

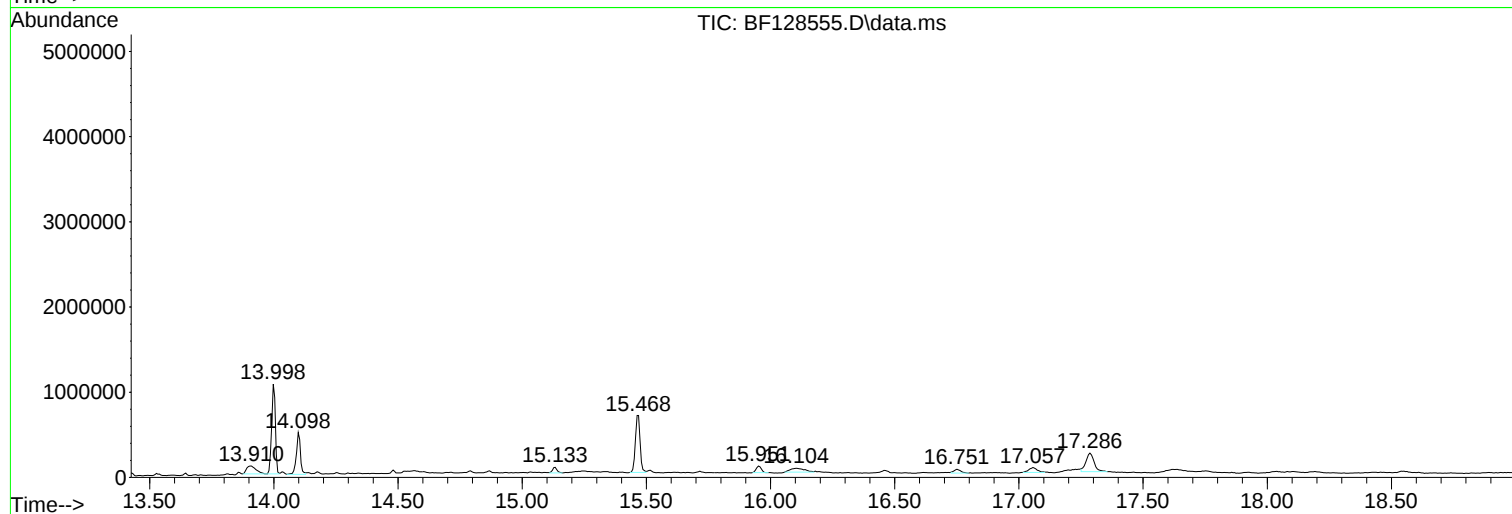
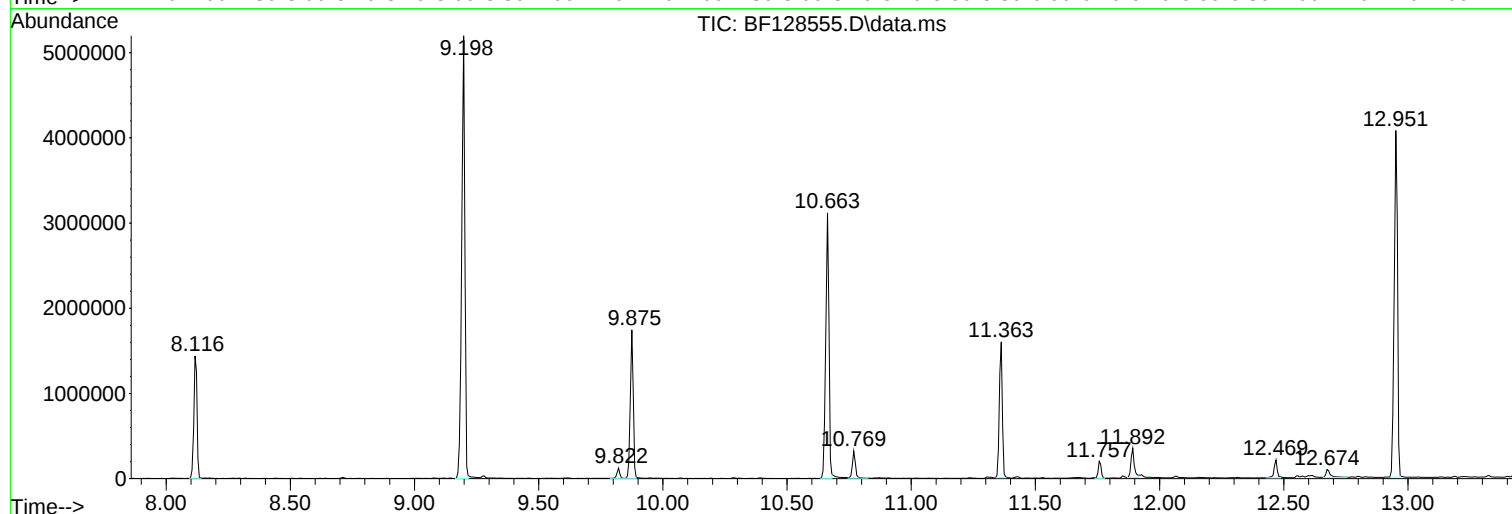
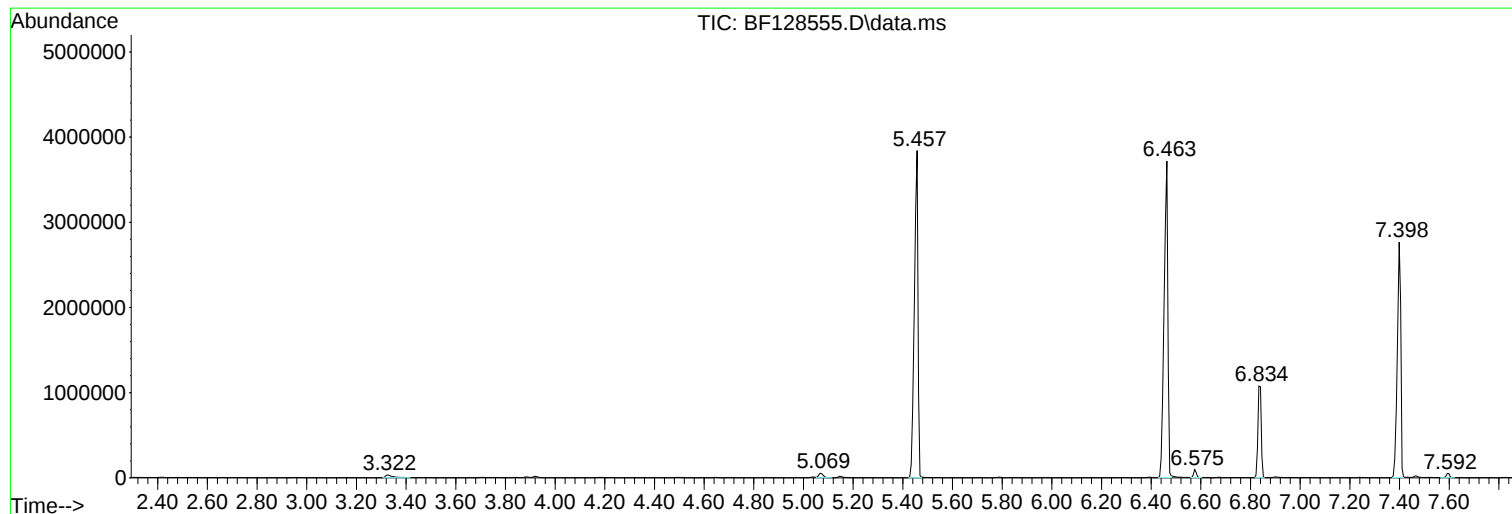
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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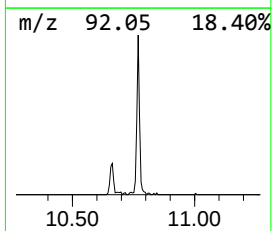
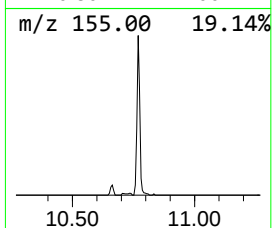
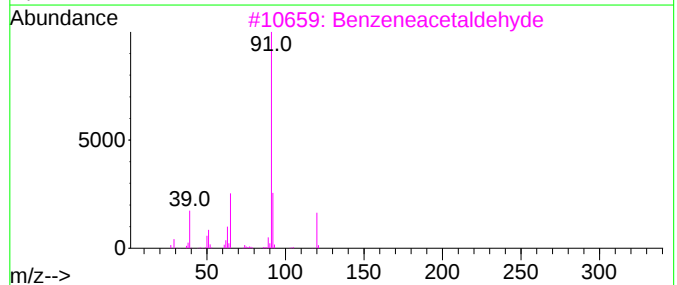
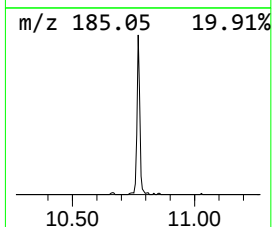
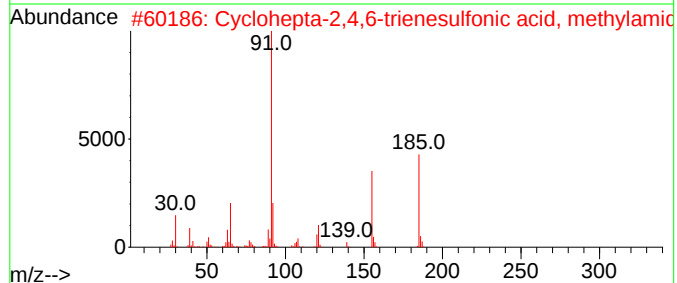
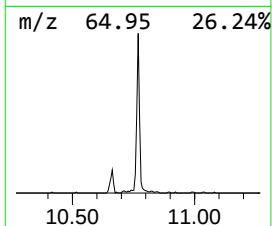
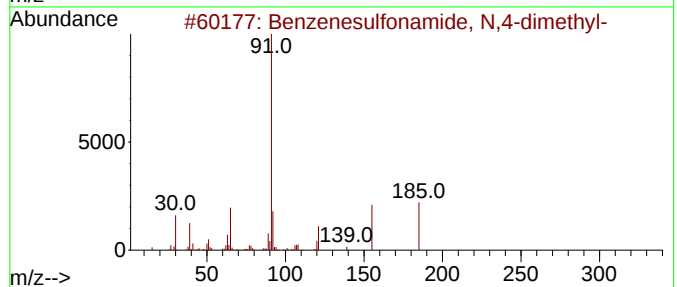
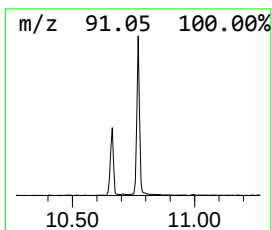
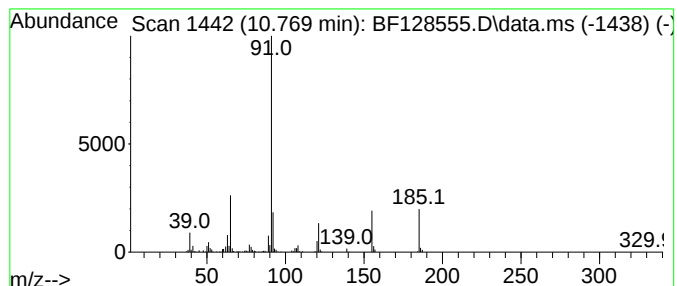
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	3.97 ng	266634	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			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	52
3			Benzeneacetaldehyde	120	C8H8O	000122-78-1	50
4			Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	50
5			Pyridine-2-carbonitrile, 3,5,6-t...	375	C13H8Cl3N3O2S	255713-77-0	47



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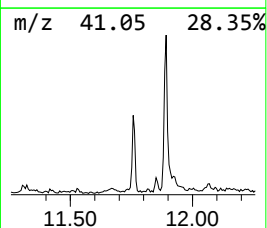
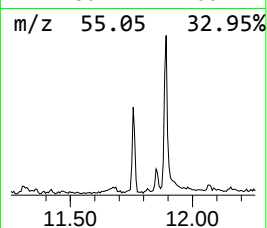
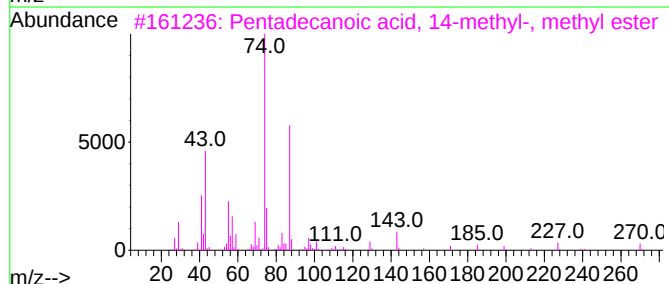
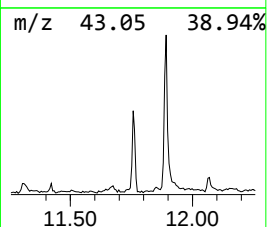
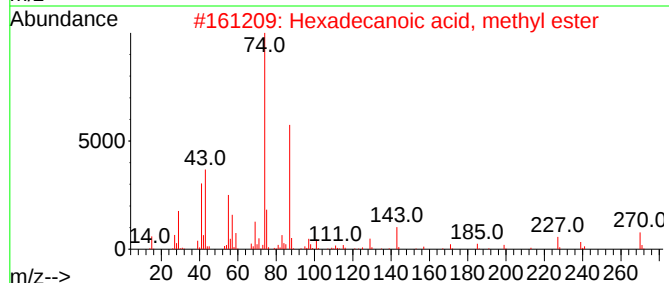
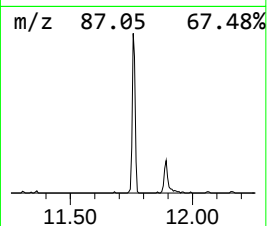
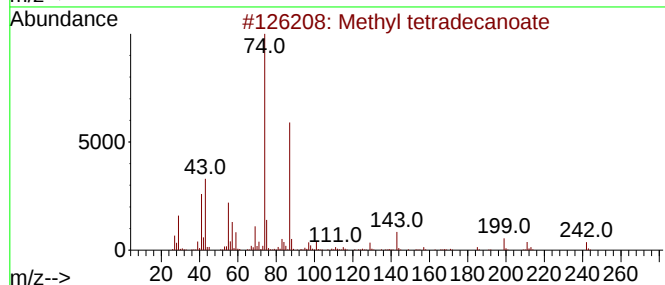
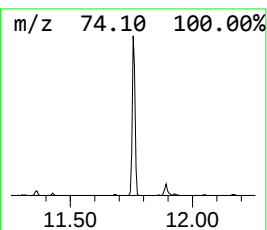
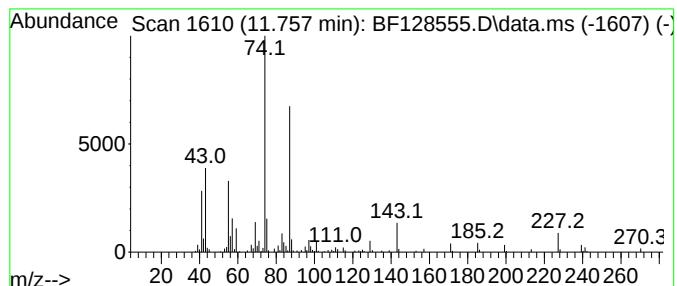
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Methyl tetradecanoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.757	2.46 ng	165217	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl tetradecanoate	242	C15H30O2	000124-10-7	95
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	91
5			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91



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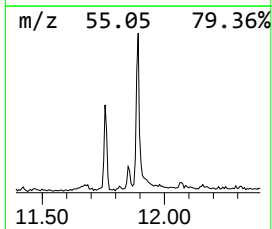
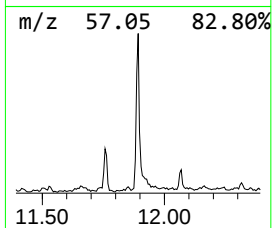
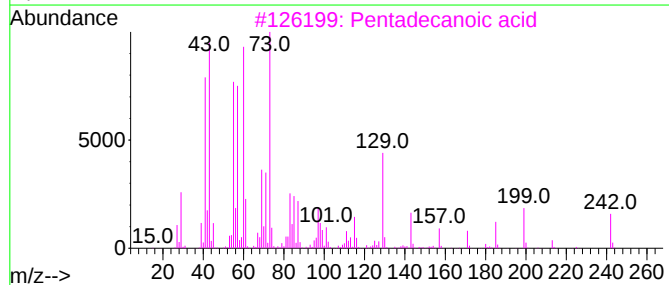
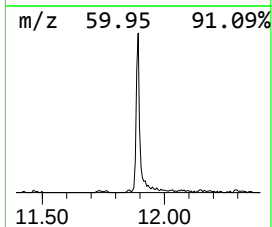
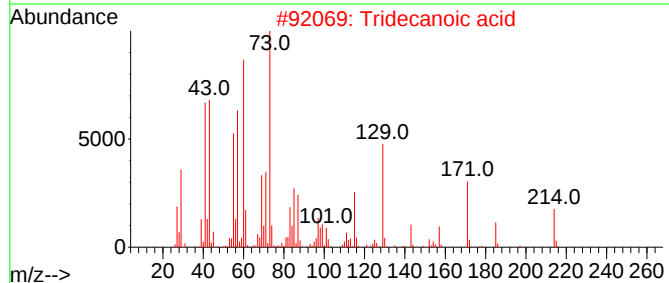
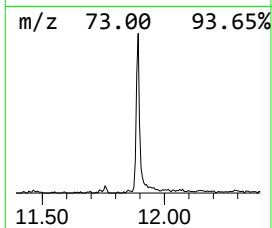
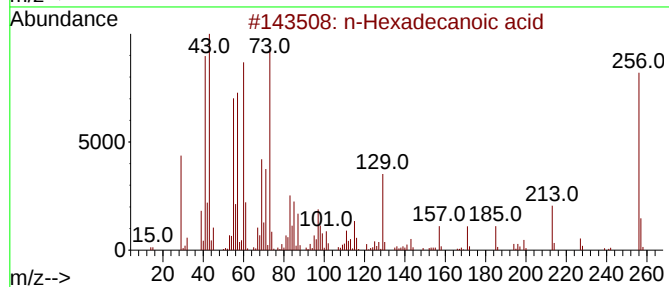
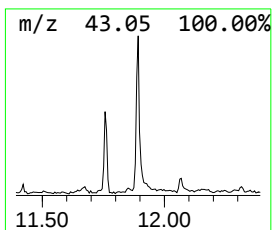
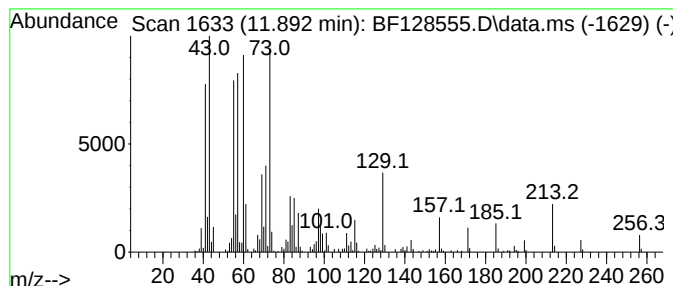
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.73 ng	317789	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	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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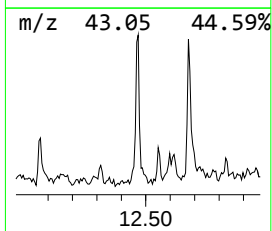
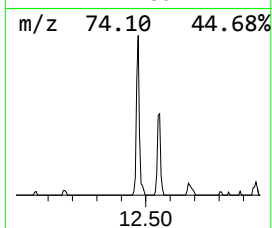
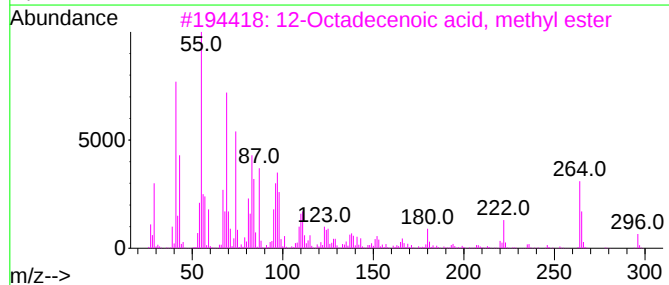
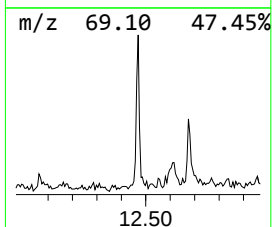
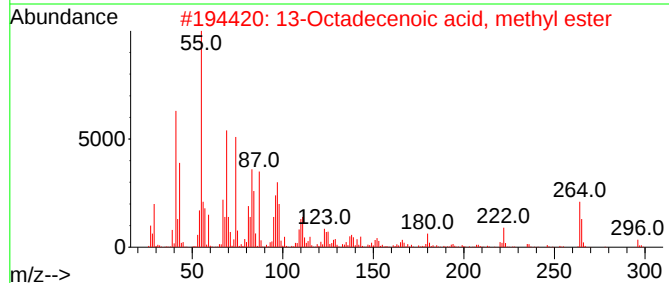
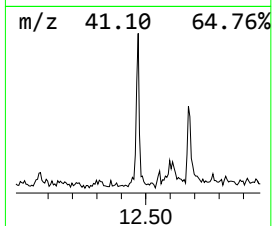
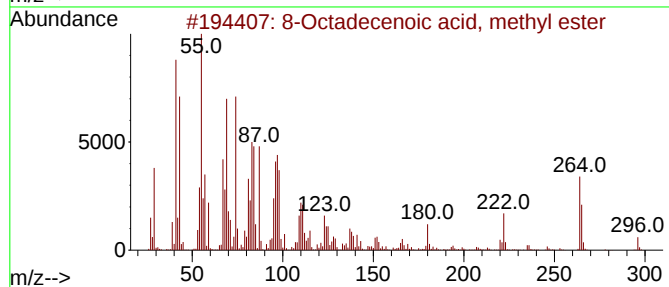
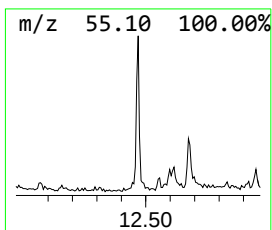
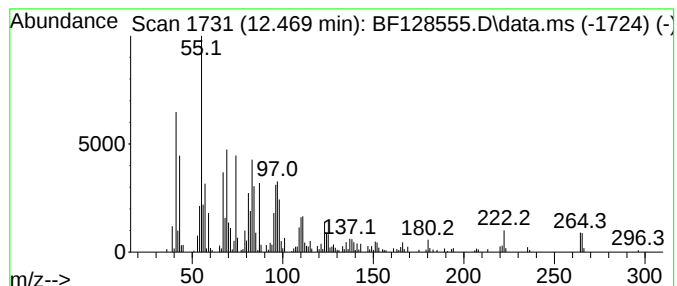
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Peak Number 4 8-Octadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.469	2.82 ng	189628	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	8-Octadecenoic acid, methyl ester		296	C19H36O2	002345-29-1	99
2	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	99
3	12-Octadecenoic acid, methyl ester		296	C19H36O2	056554-46-2	99
4	11-Octadecenoic acid, methyl ester		296	C19H36O2	052380-33-3	98
5	7-Octadecenoic acid, methyl ester		296	C19H36O2	057396-98-2	97



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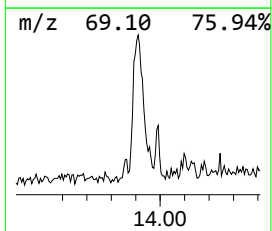
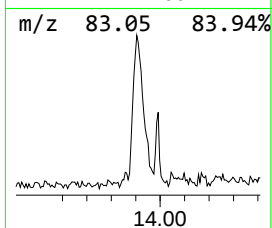
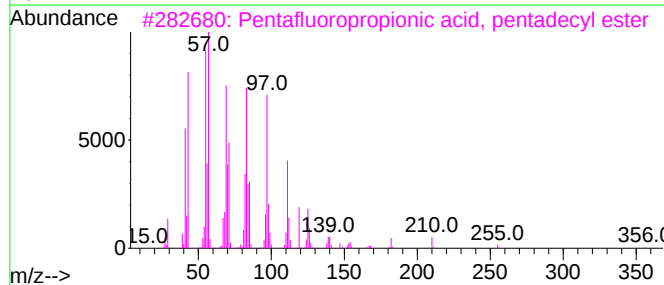
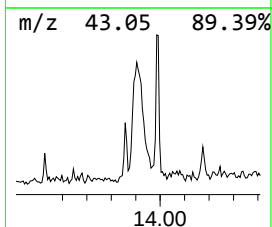
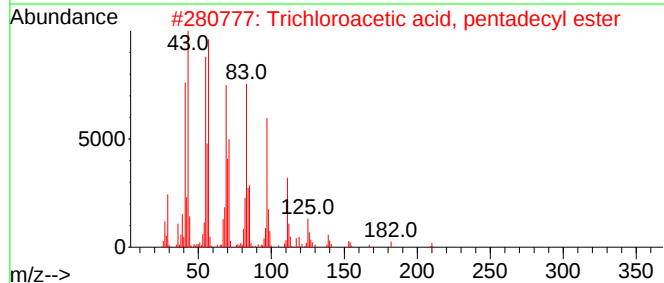
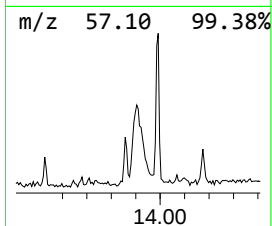
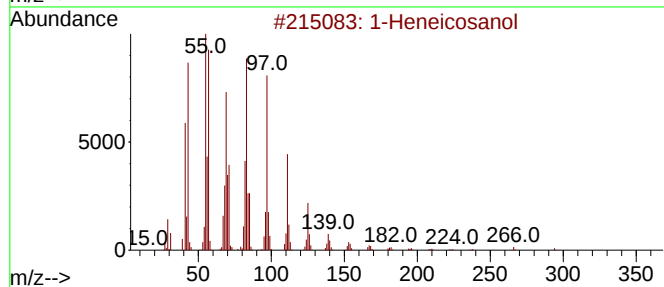
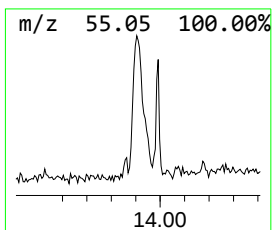
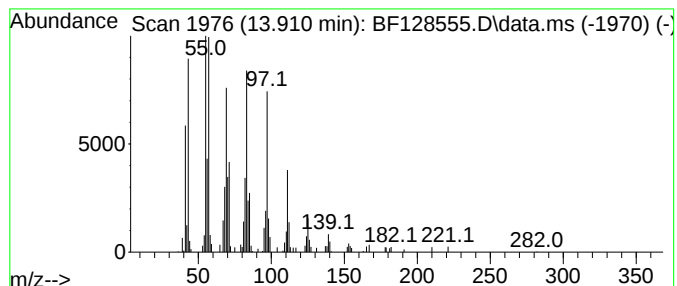
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	4.61 ng	251379	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



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P023-SS004-0006-01

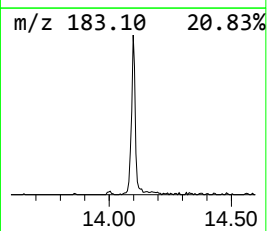
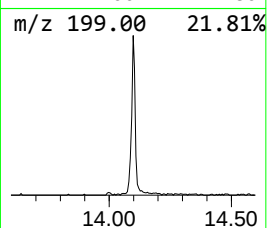
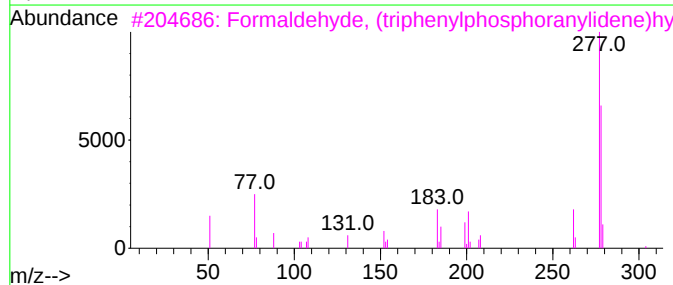
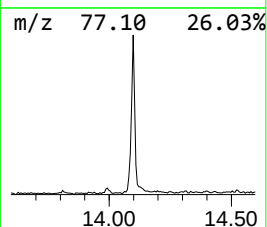
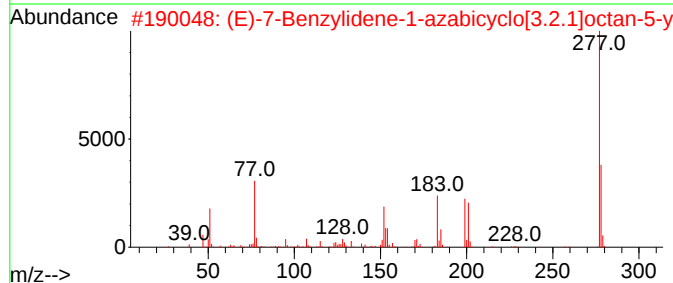
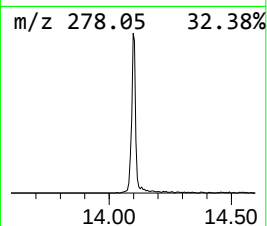
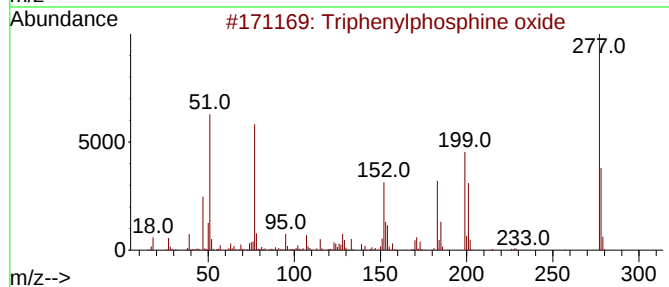
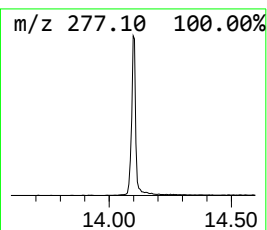
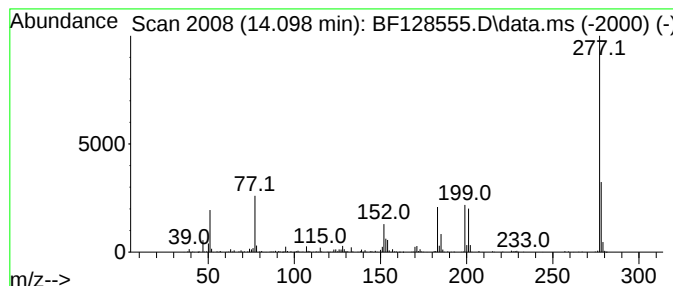
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	10.19 ng	555401	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128555.D
Acq On : 28 May 2022 18:38
Operator : CG\JU
Sample : N2933-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS004-0006-01

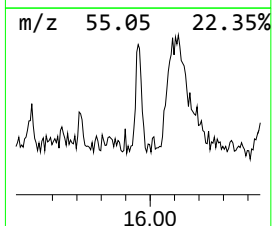
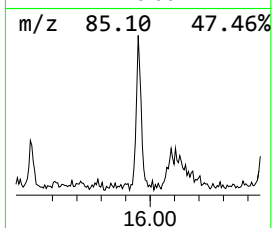
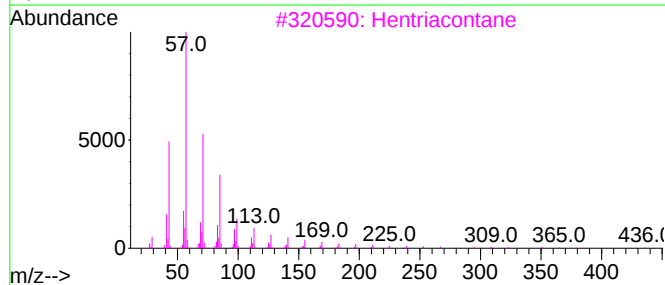
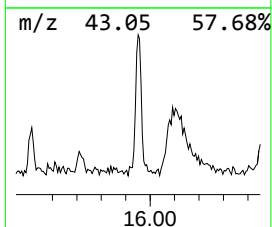
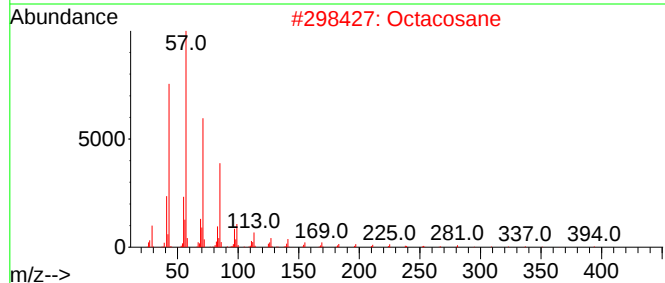
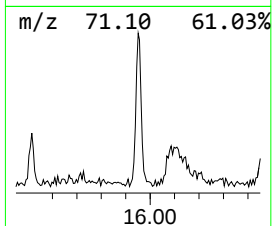
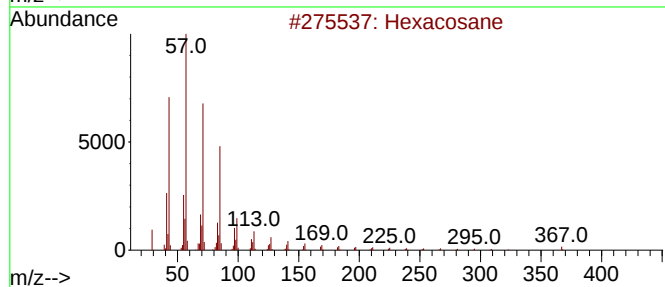
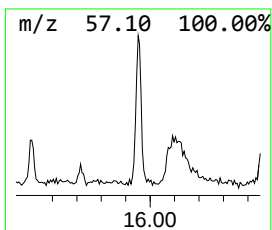
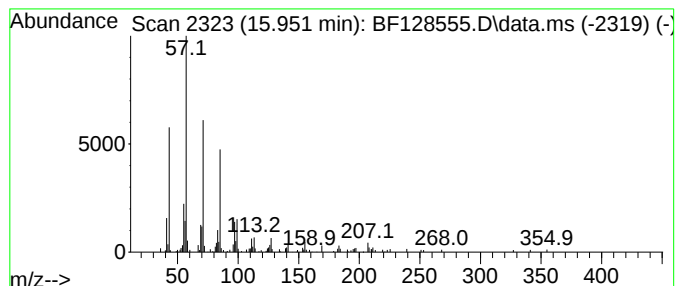
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.48 ng	111183	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Docosane	310	C22H46	000629-97-0	83
5			Eicosane	282	C20H42	000112-95-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128555.D
Acq On : 28 May 2022 18:38
Operator : CG\JU
Sample : N2933-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

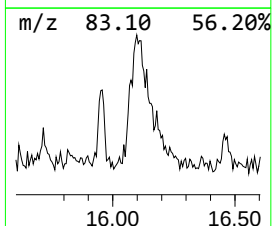
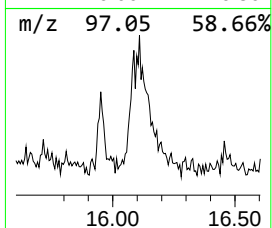
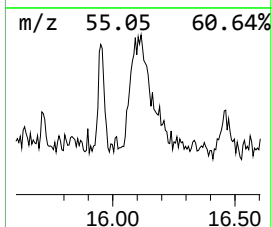
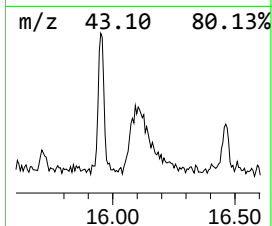
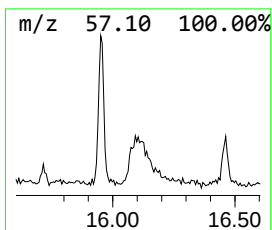
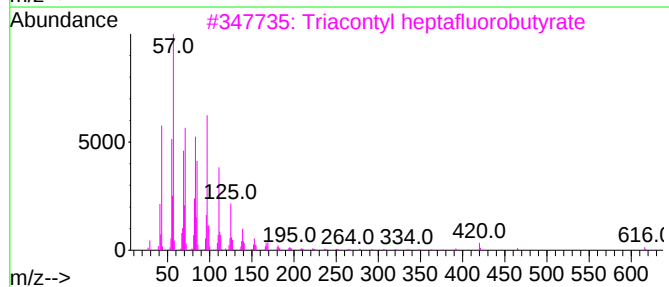
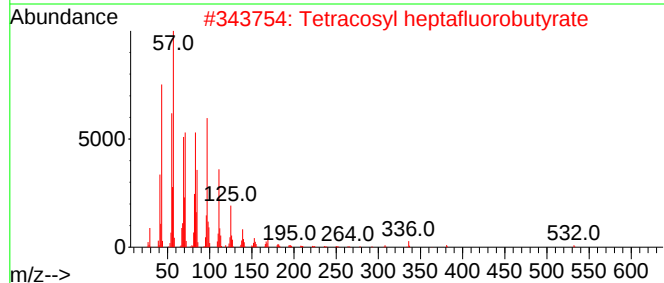
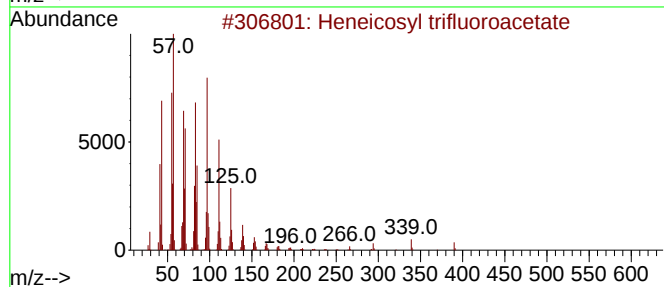
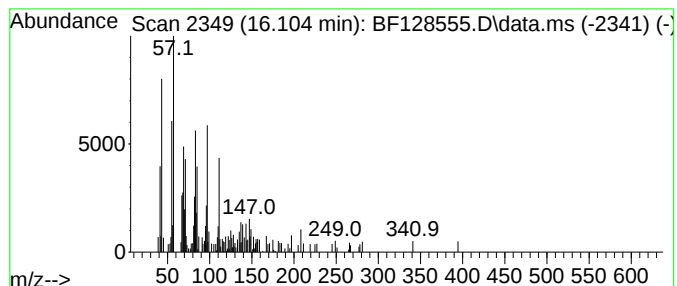
Instrument :
BNA_F
ClientSampleId :
P023-SS004-0006-01

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

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

Peak Number 8 Heneicosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.104	4.12 ng	184683	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	83
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	83
3	Triacosyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	83
4	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	80
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128555.D
Acq On : 28 May 2022 18:38
Operator : CG\JU
Sample : N2933-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS004-0006-01

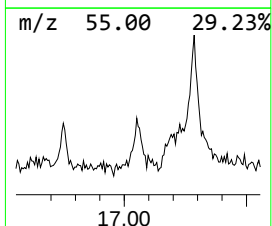
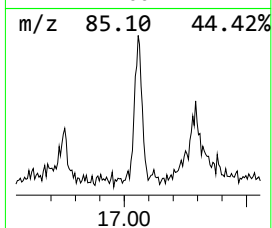
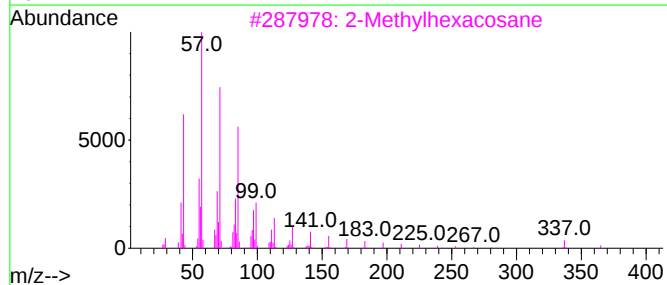
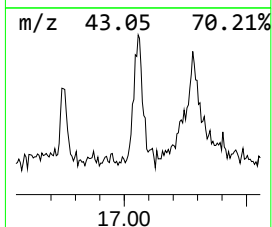
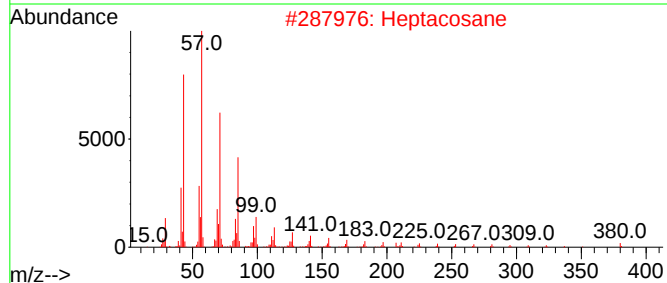
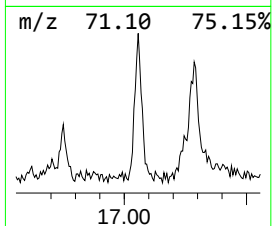
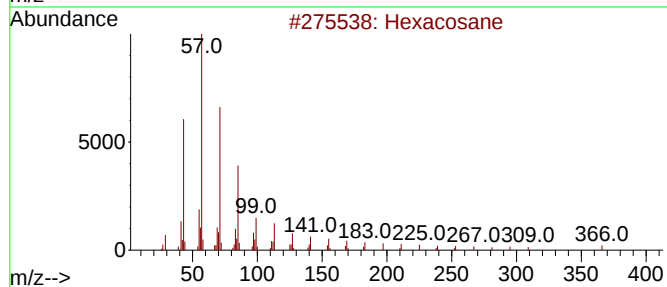
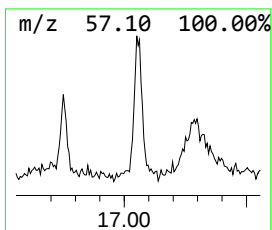
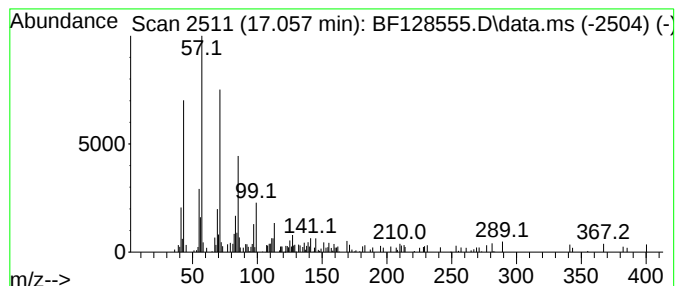
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	3.00 ng	134399	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	74
2			Heptacosane	380	C27H56	000593-49-7	74
3			2-Methylhexacosane	380	C27H56	001561-02-0	74
4			Pentacosane	352	C25H52	000629-99-2	74
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128555.D
Acq On : 28 May 2022 18:38
Operator : CG\JU
Sample : N2933-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS004-0006-01

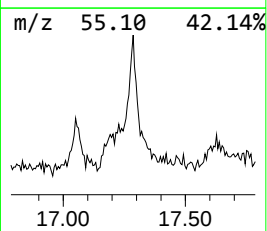
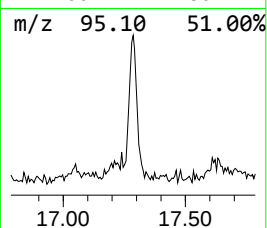
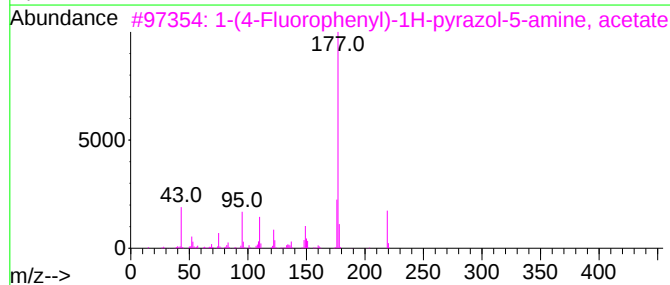
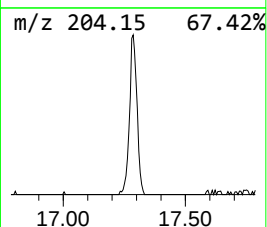
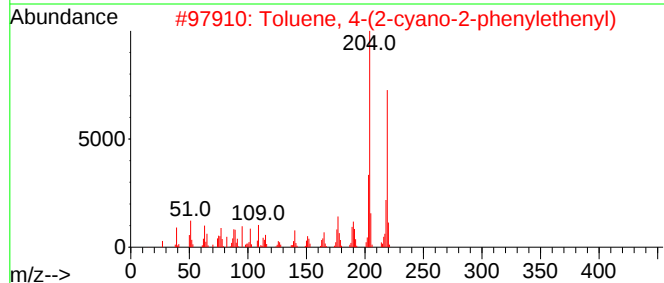
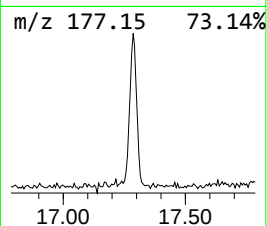
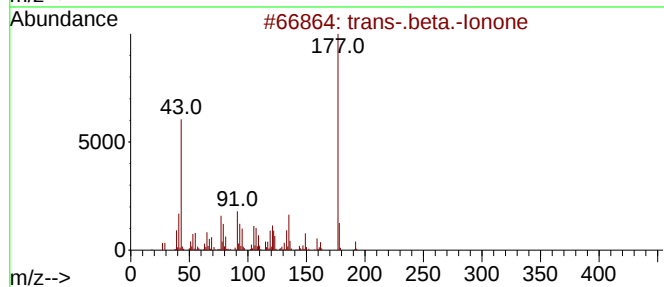
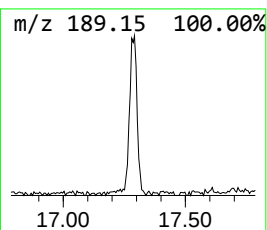
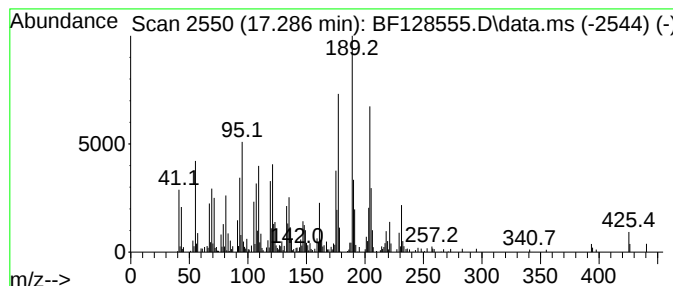
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 trans-.beta.-Ionone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	10.99 ng	492717	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		trans-.beta.-Ionone	192	C13H20O	000079-77-6	50
2		Toluene, 4-(2-cyano-2-phenylethe...	219	C16H13N	006443-76-1	38
3		1-(4-Fluorophenyl)-1H-pyrazol-5-...	219	C11H10FN3O	1000507-50-2	38
4		4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	38
5		2,3-Dimethoxy-5-aminocinnamitrile	204	C11H12N2O2	1000214-46-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128555.D
Acq On : 28 May 2022 18:38
Operator : CG\JU
Sample : N2933-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS004-0006-01

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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Methyl tetradec...	11.757	2.5	ng	165217	4	11.363	1344060	20.0
n-Hexadecanoic ...	11.892	4.7	ng	317789	4	11.363	1344060	20.0
8-Octadecenoic ...	12.469	2.8	ng	189628	4	11.363	1344060	20.0
1-Heneicosanol	13.910	4.6	ng	251379	5	13.998	1090530	20.0
Triphenylphosph...	14.098	10.2	ng	555401	5	13.998	1090530	20.0
Hexacosane	15.951	2.5	ng	111183	6	15.463	896482	20.0
Heneicosyl trif...	16.104	4.1	ng	184683	6	15.463	896482	20.0
Heptacosane	17.057	3.0	ng	134399	6	15.463	896482	20.0
trans-.beta.-Io...	17.286	11.0	ng	492717	6	15.463	896482	20.0