

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
 Data File : BF134473.D
 Acq On : 25 Jul 2023 20:50
 Operator : CG\JU
 Sample : 03647-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-1

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134473.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	3	16	21	rBV	236176	371834	11.41%	1.736%
2	5.116	511	515	522	rBV2	23065	33560	1.03%	0.157%
3	5.481	573	577	580	rBV	3348547	3191078	97.88%	14.898%
4	6.481	742	747	750	rBV	2885623	3260247	100.00%	15.221%
5	6.833	803	807	815	rBV	742036	648590	19.89%	3.028%
6	7.398	899	903	906	rBV	2091773	2069998	63.49%	9.664%
7	8.110	1021	1024	1033	rBV	1042736	812011	24.91%	3.791%
8	9.192	1203	1208	1211	rBV	3343423	3006772	92.23%	14.038%
9	9.586	1271	1275	1279	rBV	105037	96553	2.96%	0.451%
10	9.869	1319	1323	1326	rBV	935617	728114	22.33%	3.399%
11	10.663	1454	1458	1462	rBV	1847380	1766558	54.18%	8.248%
12	11.363	1573	1577	1580	rBV	643221	528536	16.21%	2.468%
13	11.892	1664	1667	1675	rBV3	176854	184725	5.67%	0.862%
14	12.586	1782	1785	1788	rBV	48927	45466	1.39%	0.212%
15	12.686	1799	1802	1808	rBV3	27291	38025	1.17%	0.178%
16	12.815	1819	1824	1828	rVB	52544	50973	1.56%	0.238%
17	12.963	1844	1849	1852	rBV	2679376	2370674	72.71%	11.068%
18	13.874	1999	2004	2013	rBV2	128805	309619	9.50%	1.446%
19	14.027	2025	2030	2033	rBV	488076	508194	15.59%	2.373%
20	14.115	2042	2045	2050	rBV7	21819	35338	1.08%	0.165%
21	14.486	2105	2108	2111	rBV	329109	297373	9.12%	1.388%
22	14.521	2111	2114	2120	rVB2	96091	168582	5.17%	0.787%
23	14.798	2159	2161	2167	rVB2	33689	41518	1.27%	0.194%
24	14.951	2180	2187	2191	rBV2	86349	128799	3.95%	0.601%
25	15.145	2217	2220	2224	rVB	129532	152357	4.67%	0.711%
26	15.209	2227	2231	2233	rBV5	32898	55141	1.69%	0.257%
27	15.527	2280	2285	2295	rBV	240198	328356	10.07%	1.533%
28	15.756	2320	2324	2329	rVB	53475	71600	2.20%	0.334%
29	15.998	2363	2365	2368	rVB3	36999	35757	1.10%	0.167%
30	16.127	2383	2387	2391	rBV5	25423	34419	1.06%	0.161%
31	18.544	2791	2798	2799	rBV6	24222	48250	1.48%	0.225%

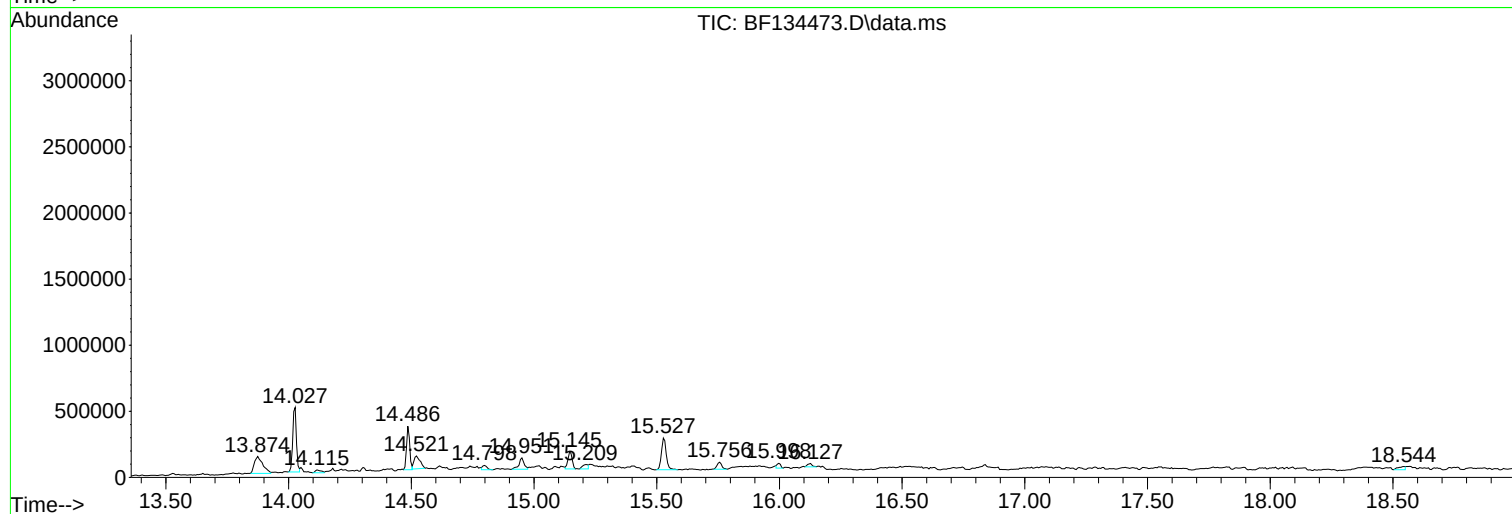
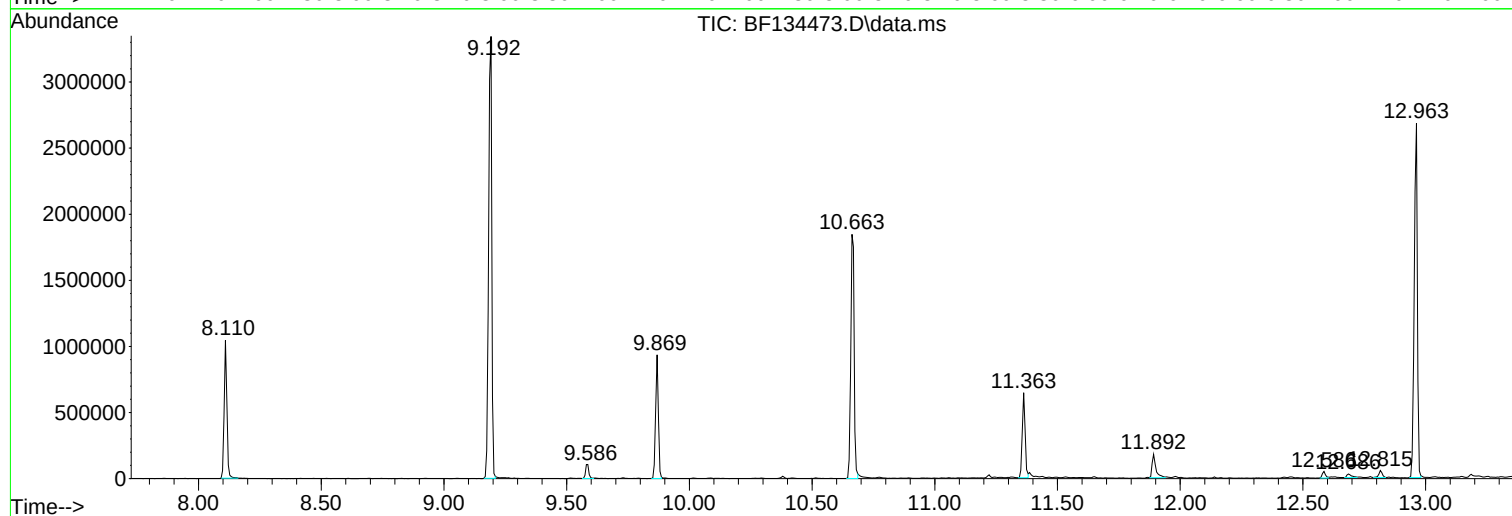
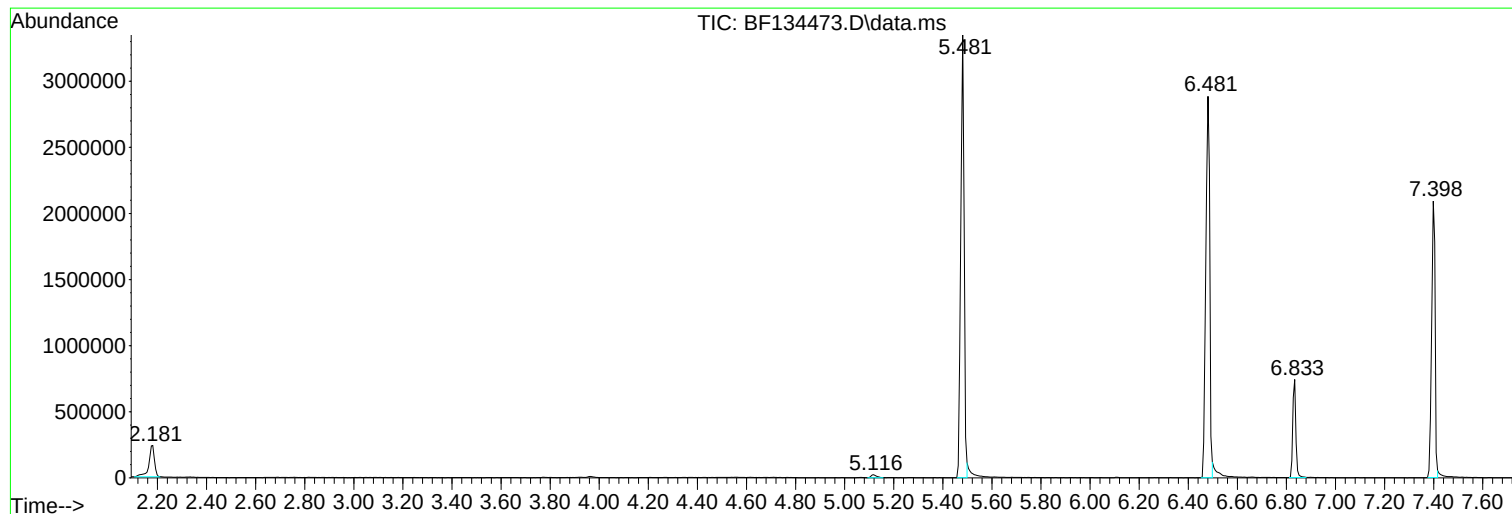
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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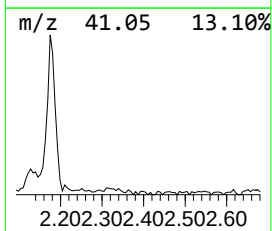
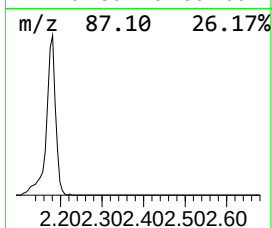
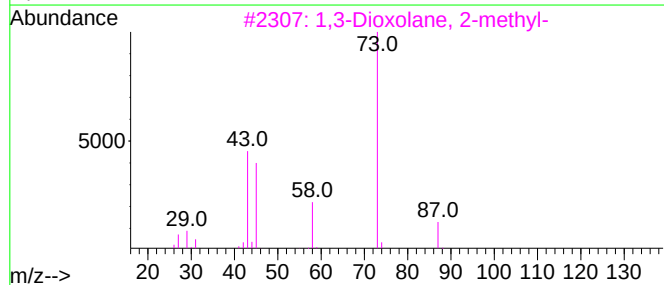
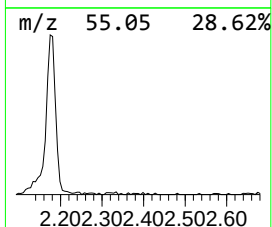
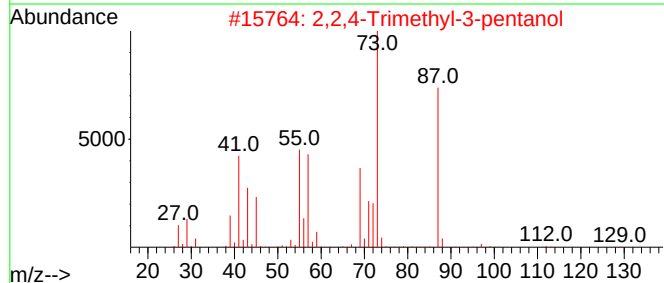
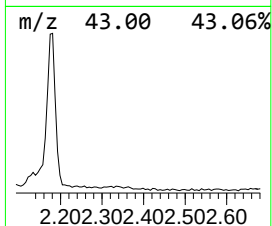
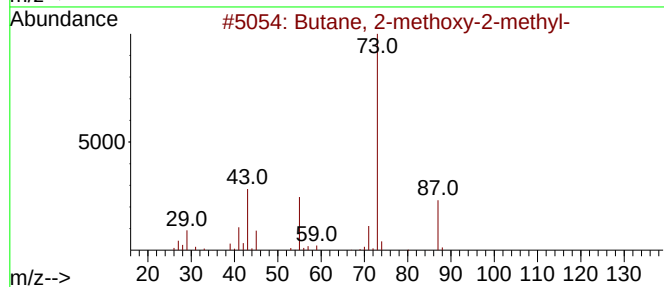
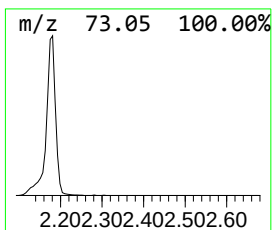
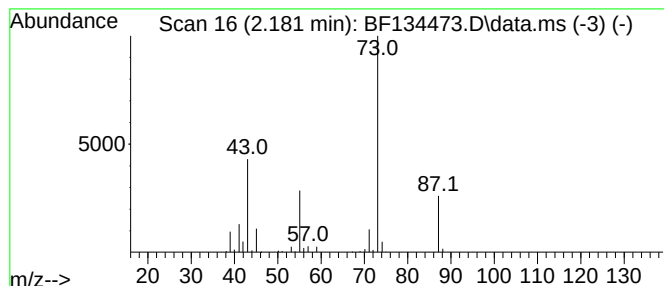
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	11.47 ng	371834	1,4-Dichlorobenzene-d4	6.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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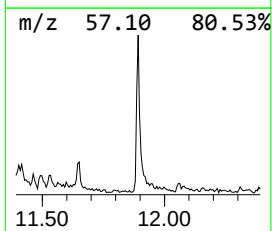
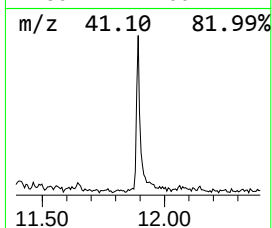
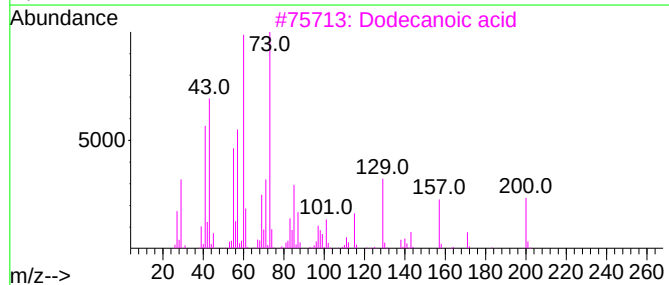
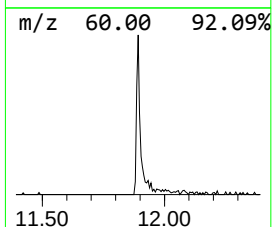
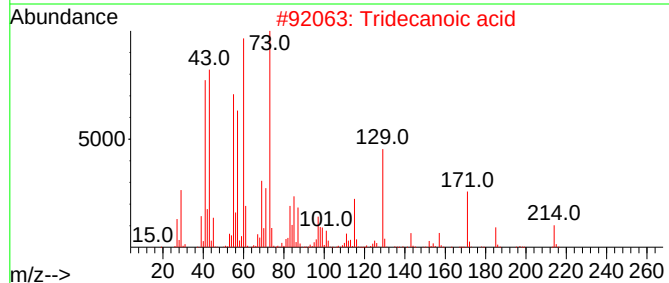
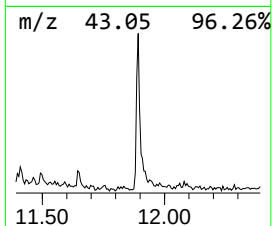
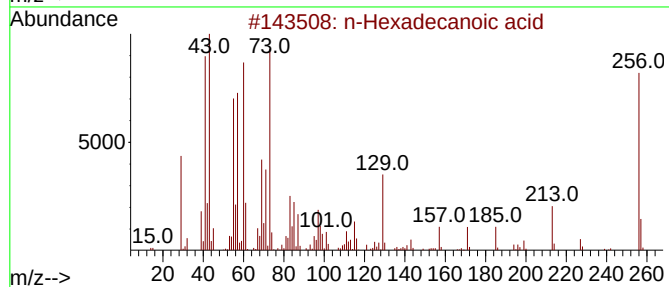
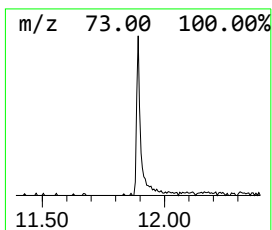
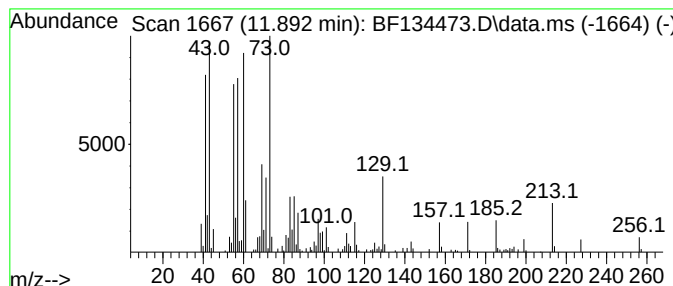
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	6.99 ng	184725	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	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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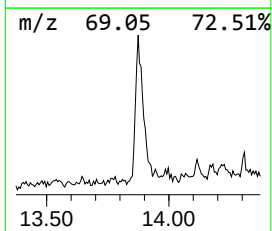
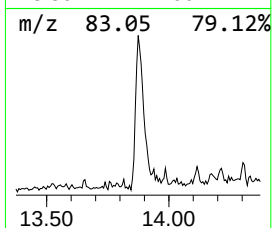
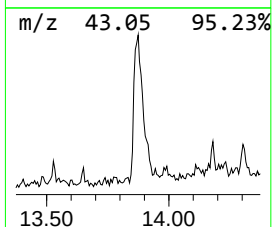
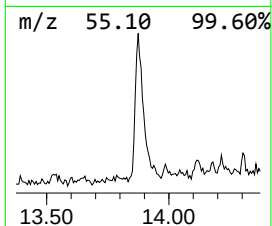
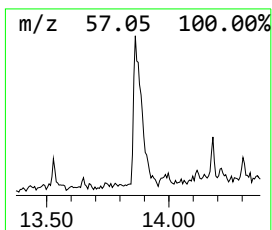
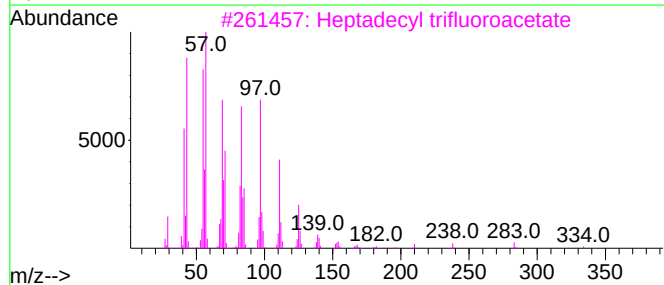
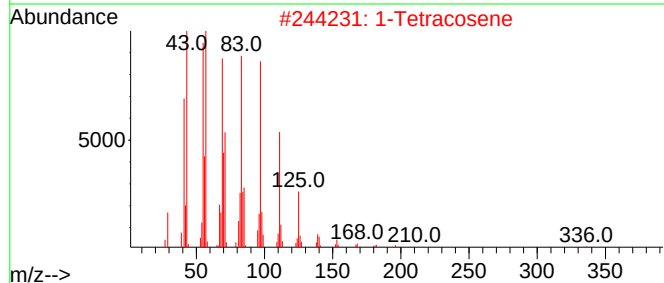
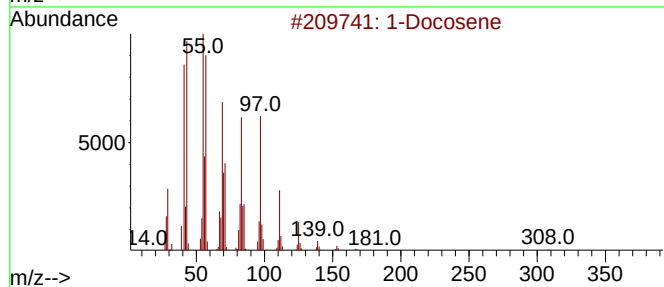
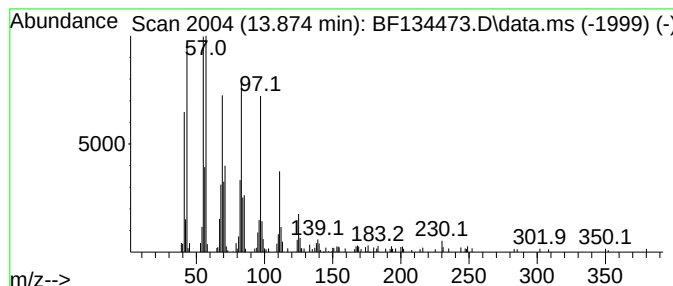
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	12.19 ng	309619	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	97
2	1-Tetracosene			336	C24H48	010192-32-2	95
3	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	95
4	1-Heneicosanol			312	C21H44O	015594-90-8	95
5	Octadecyl trifluoroacetate			366	C20H37F3O2	079392-43-1	94



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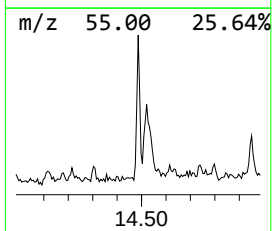
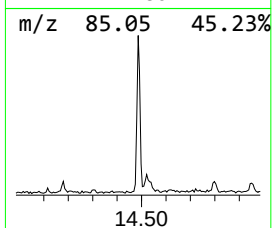
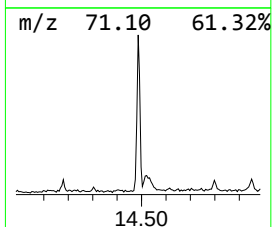
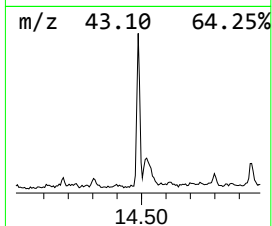
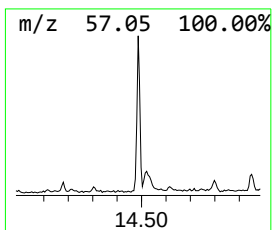
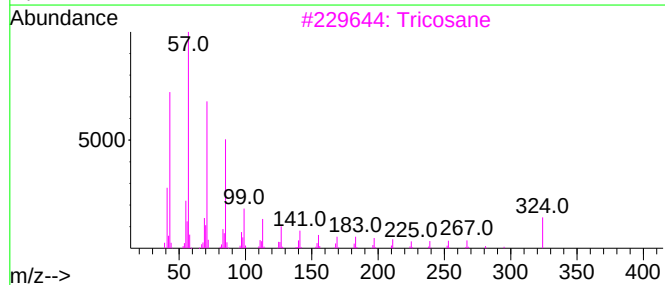
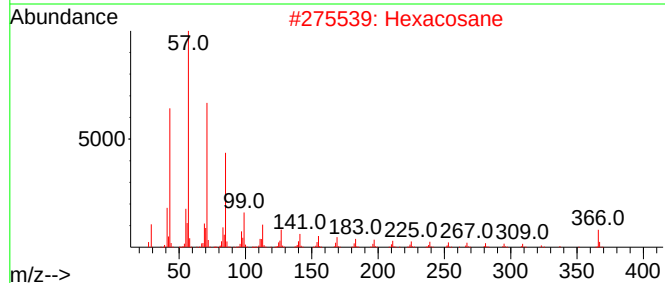
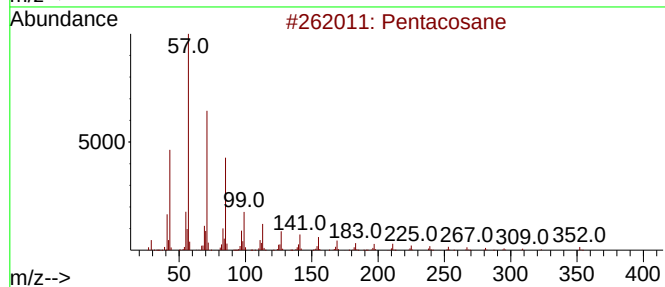
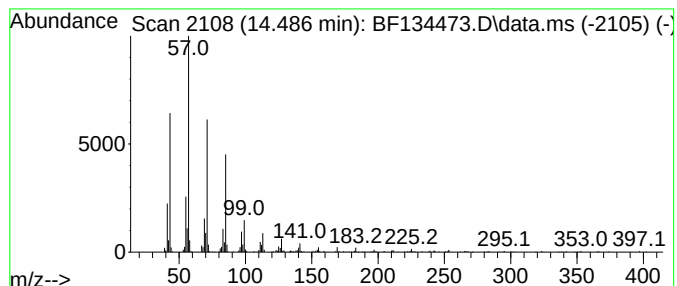
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	11.70 ng	297373	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	95
2			Hexacosane	366	C26H54	000630-01-3	94
3			Tricosane	324	C23H48	000638-67-5	94
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	94



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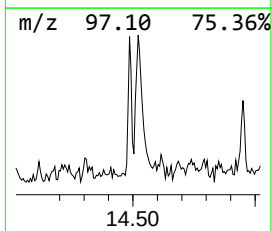
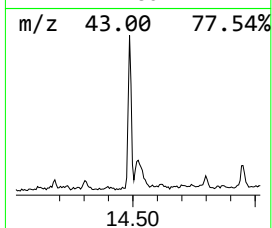
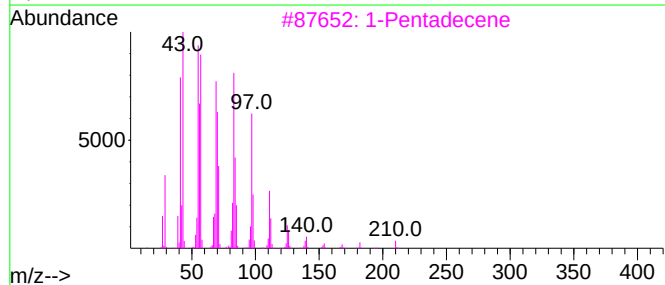
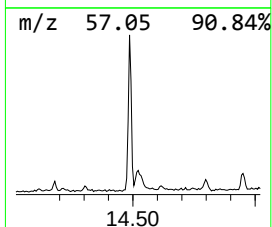
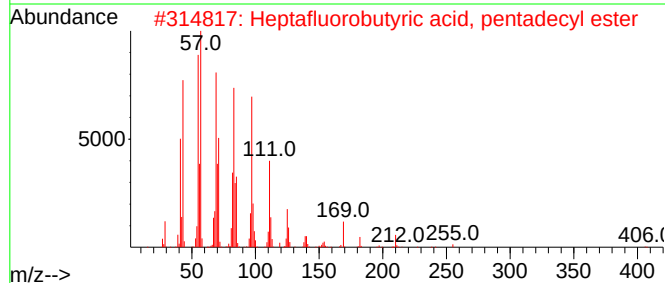
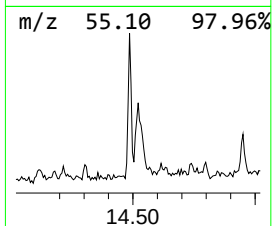
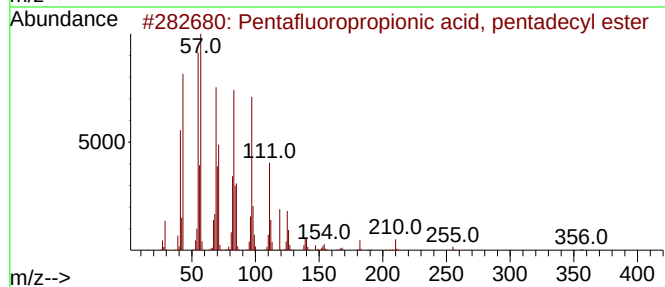
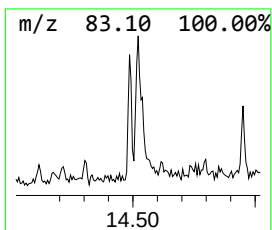
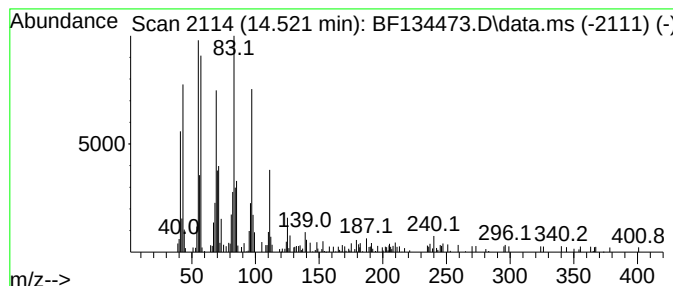
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	6.63 ng	168582	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			1-Pentadecene	210	C15H30	013360-61-7	90
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



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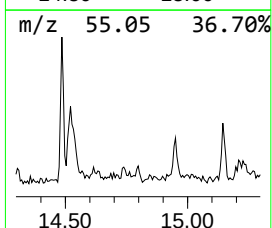
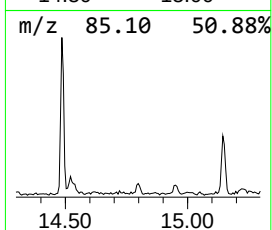
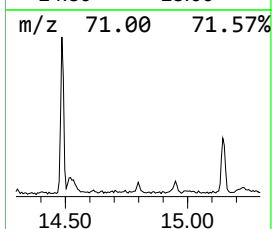
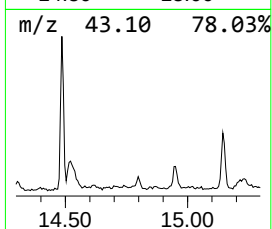
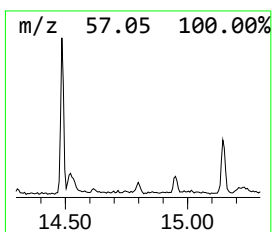
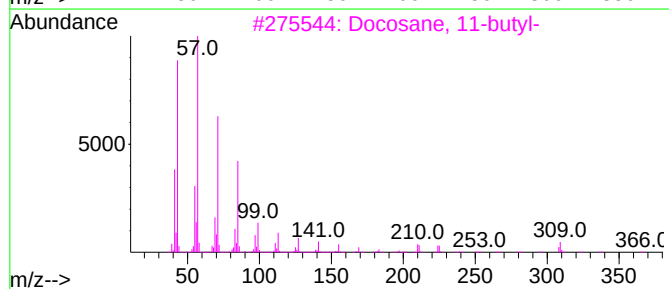
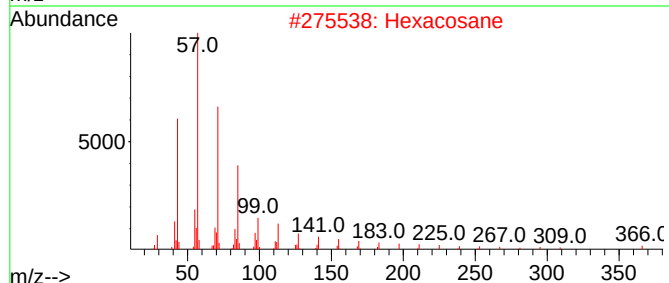
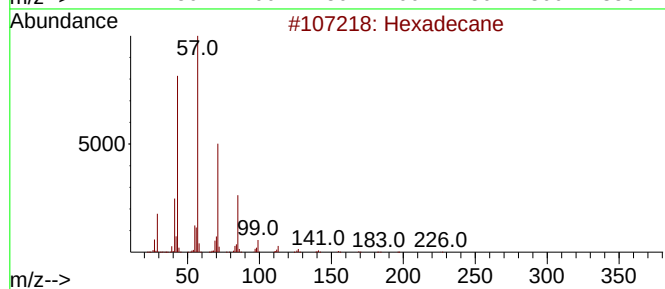
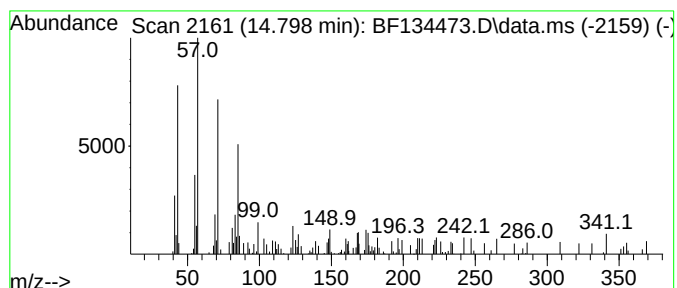
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	2.53 ng	41518	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	53
2			Hexacosane	366	C26H54	000630-01-3	52
3			Docosane, 11-butyl-	366	C26H54	013475-76-8	52
4			Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	49
5			Triacontane	422	C30H62	000638-68-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
Operator : CG\JU
Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SAMPLE-1

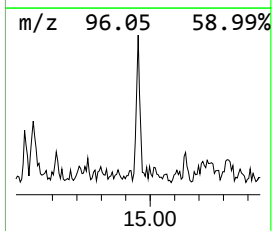
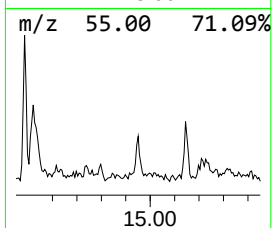
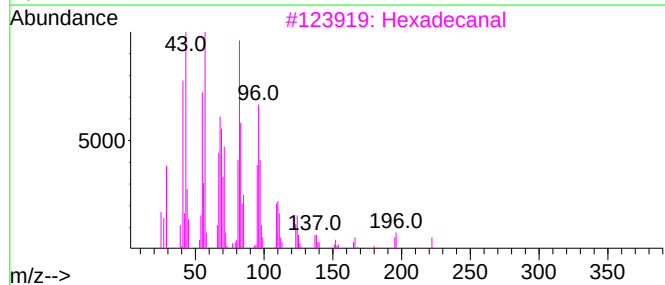
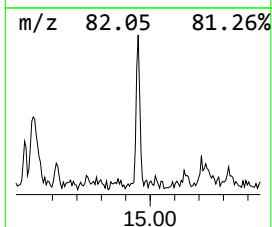
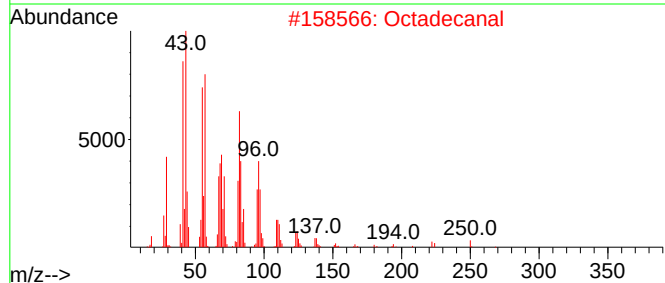
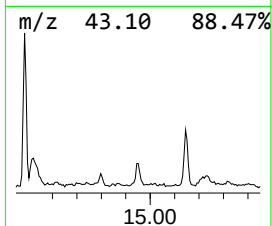
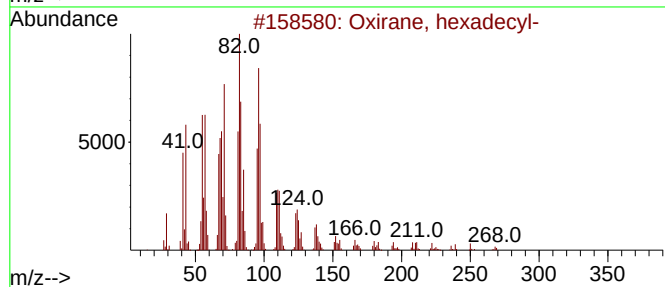
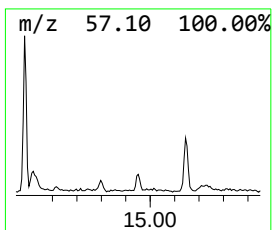
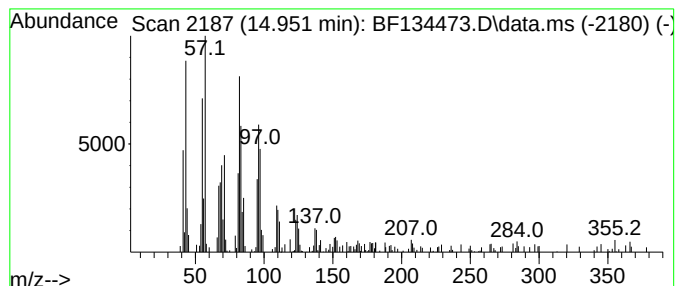
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.951	7.85 ng	128799	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	97
2			Octadecanal	268	C18H36O	000638-66-4	94
3			Hexadecanal	240	C16H32O	000629-80-1	91
4			Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	90
5			Tricosanal	338	C23H46O	072934-02-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
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Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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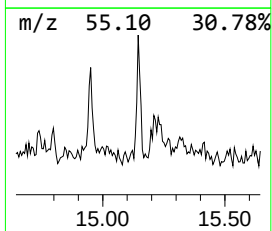
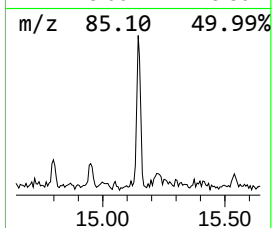
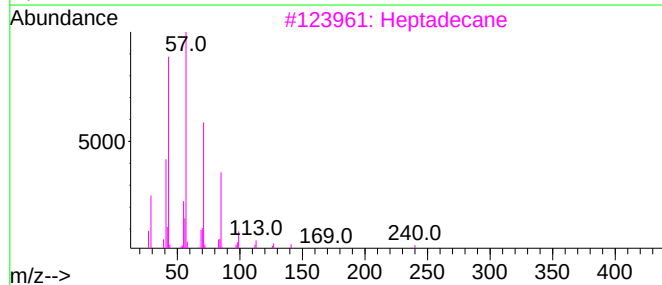
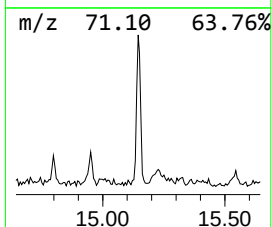
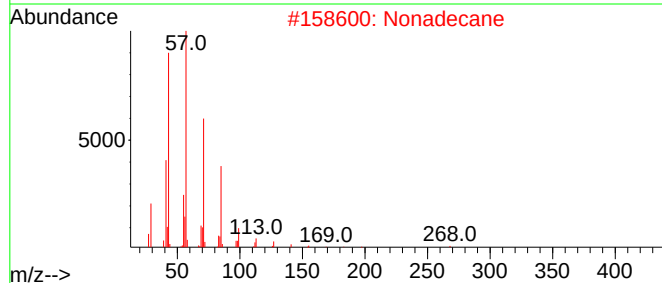
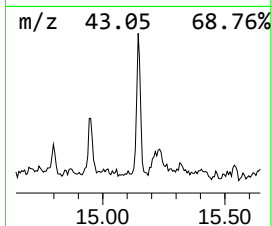
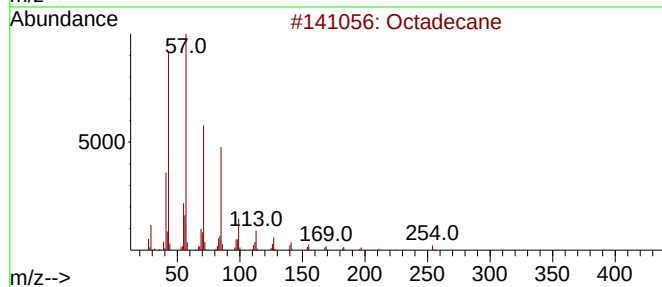
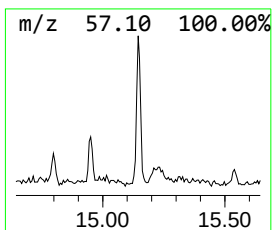
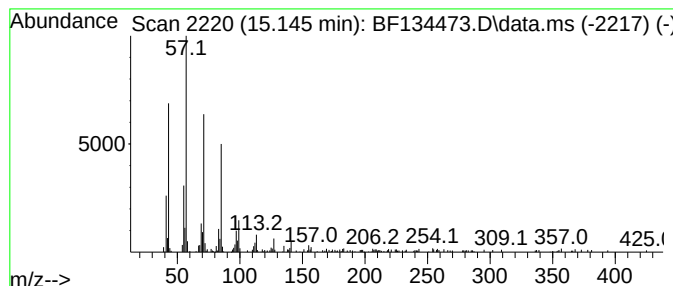
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	9.28 ng	152357	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	96
2			Nonadecane	268	C19H40	000629-92-5	95
3			Heptadecane	240	C17H36	000629-78-7	94
4			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
Operator : CG\JU
Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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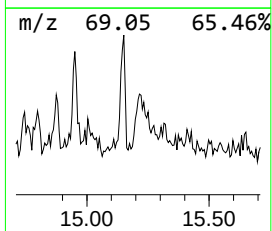
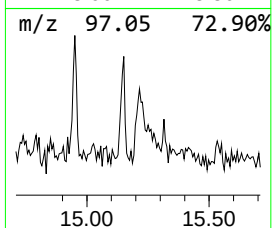
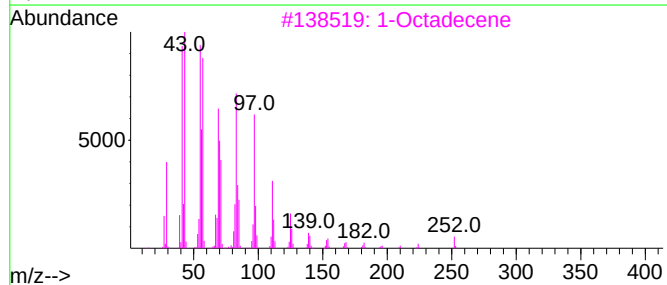
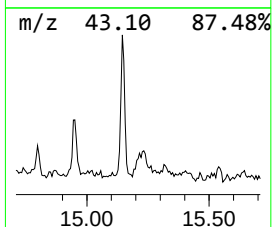
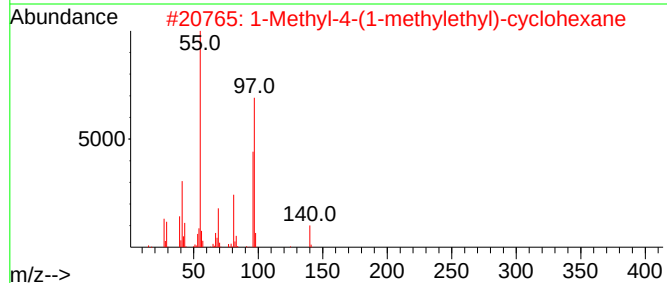
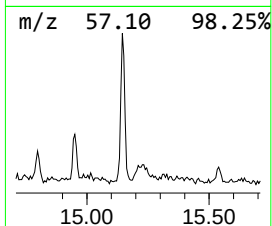
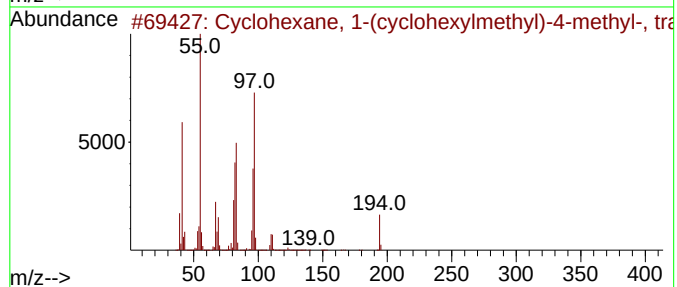
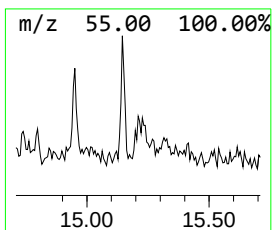
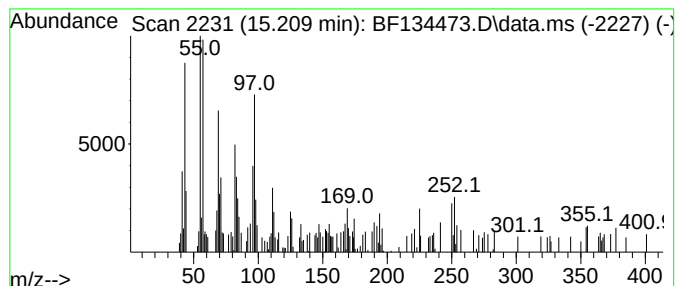
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.209 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.209	3.36 ng	55141	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-98-2	41
2			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	38
3			1-Octadecene	252	C18H36	000112-88-9	38
4			Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	38
5			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
Operator : CG\JU
Sample : 03647-01
Misc :
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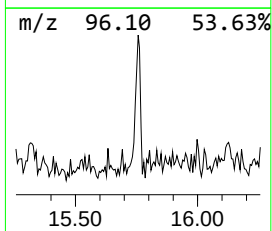
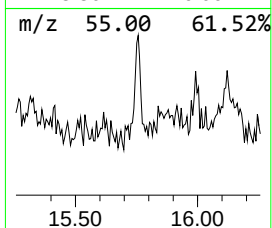
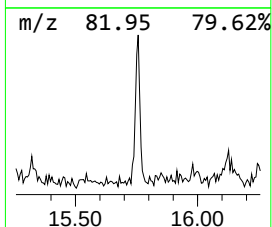
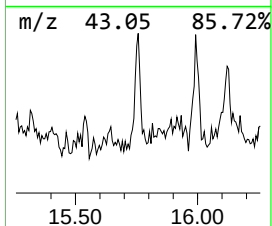
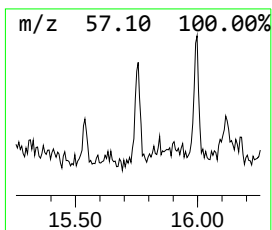
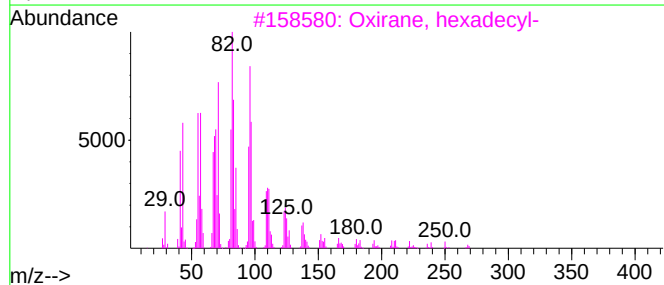
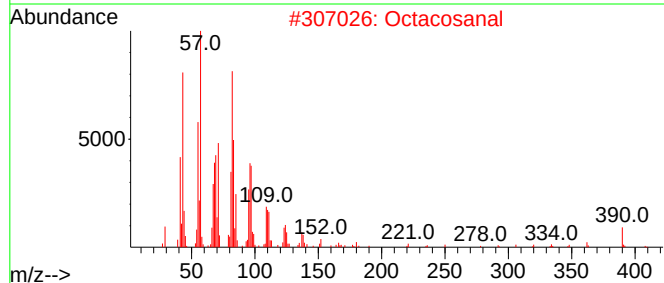
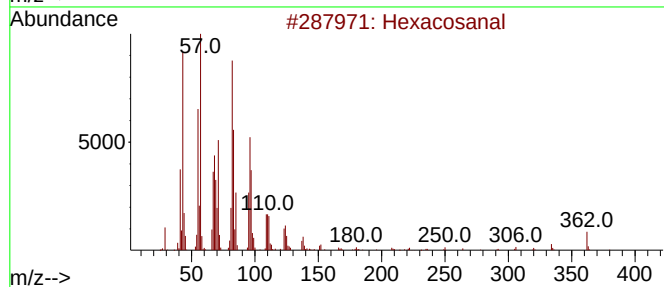
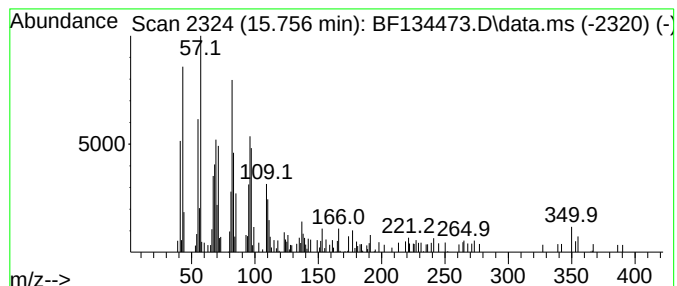
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.756	4.36 ng	71600	Perylene-d12		15.527	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosanal		380	C26H52O	026627-85-0	83
2	Octacosanal		408	C28H56O	022725-64-0	83
3	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	80
4	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	74
5	Eicosanal-		296	C20H40O	002400-66-0	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
Operator : CG\JU
Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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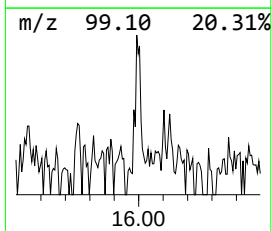
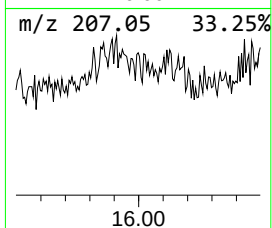
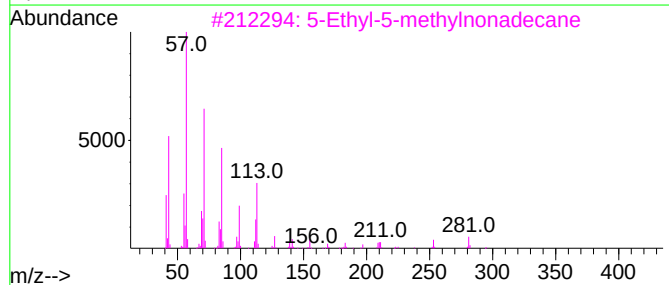
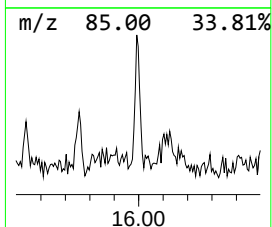
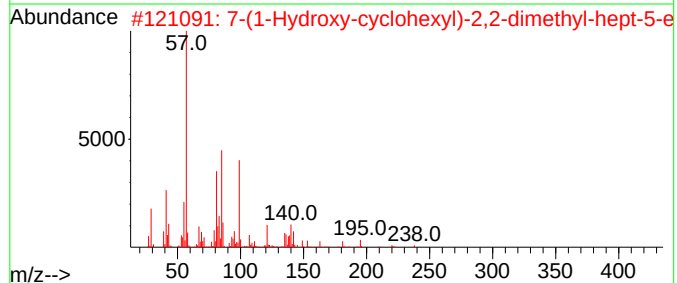
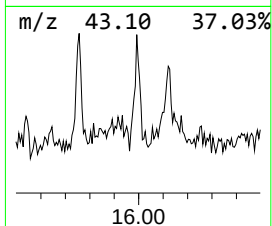
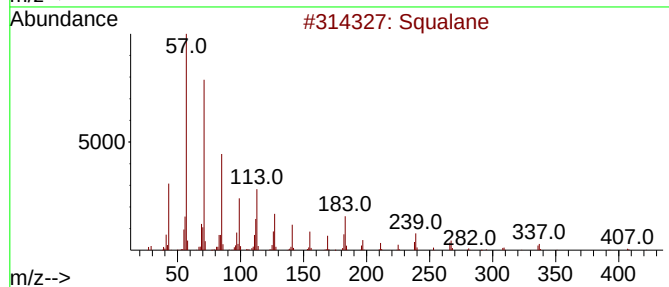
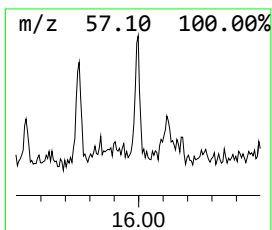
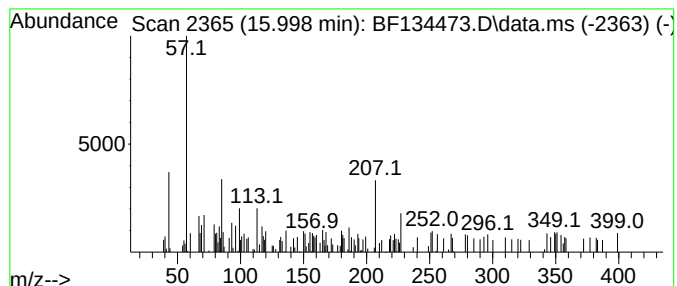
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown15.998 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.18 ng	35757	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalane	422	C30H62	000111-01-3	25
2			7-(1-Hydroxy-cyclohexyl)-2,2-dim...	238	C15H26O2	083040-91-9	14
3			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	12
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	10
5			Hentriacontane	437	C31H64	000630-04-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
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Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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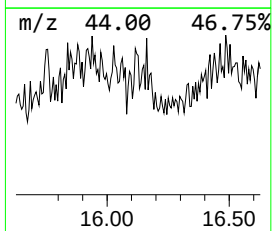
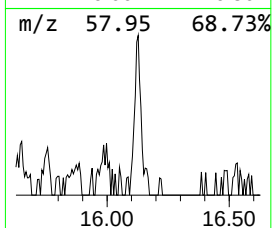
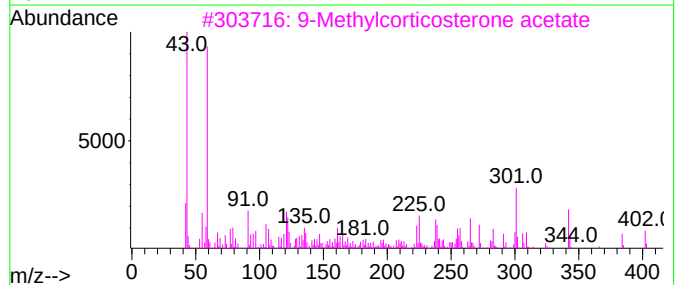
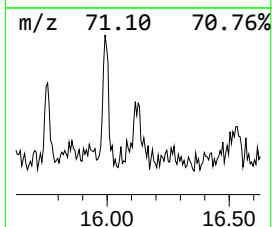
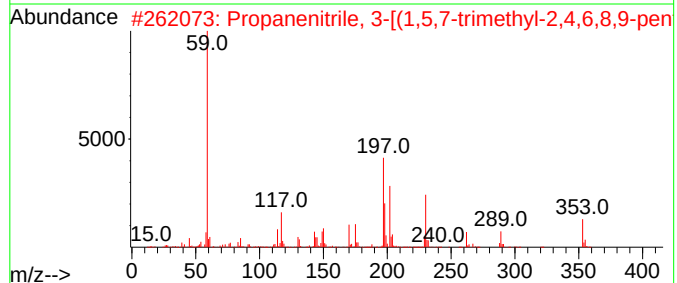
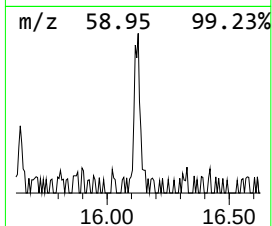
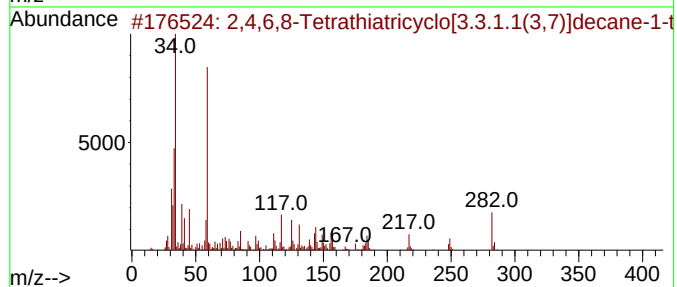
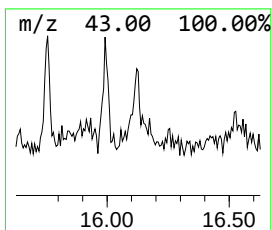
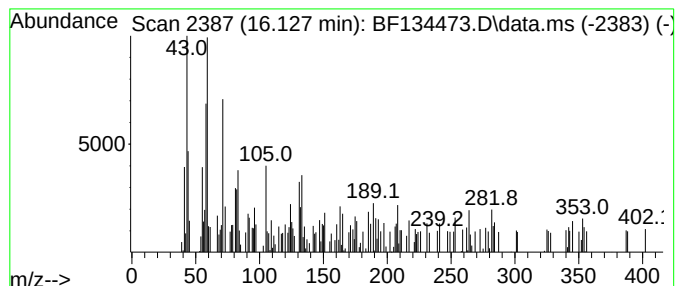
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.127 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.127	2.10 ng	34419	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6,8-Tetrathiatricyclo[3.3.1...	282	C9H14S5	057274-35-8	38		
2	Propanenitrile, 3-[(1,5,7-trimet...	353	C11H15NS6	057274-41-6	35		
3	9-Methylcorticosterone acetate	402	C24H34O5	1000128-16-0	35		
4	Propanamide, 2-methoxy-N-(1-phen...	207	C12H17NO2	1000142-13-8	35		
5	3,6,9,12-Tetraoxatetradecan-1-ol...	322	C15H34O5Si	1000352-09-6	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
Operator : CG\JU
Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1

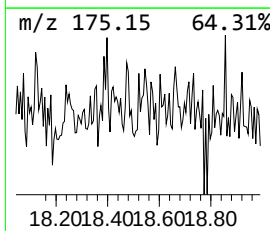
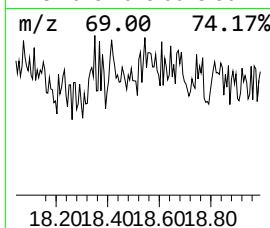
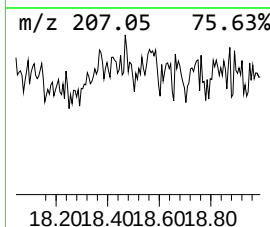
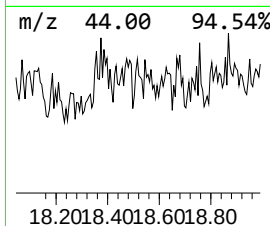
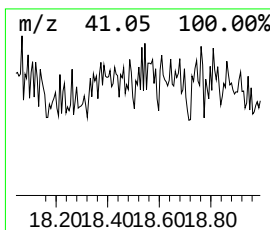
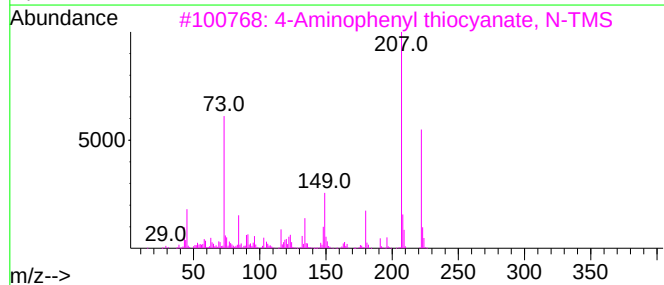
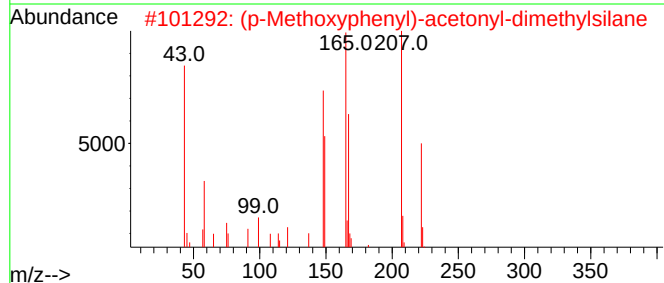
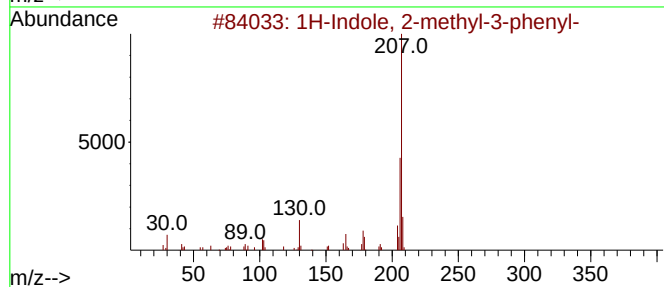
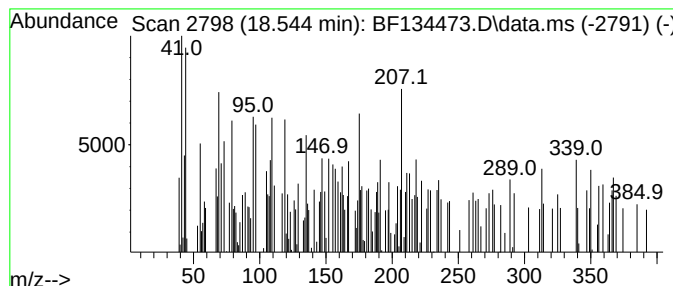
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.544 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.544	2.94 ng	48250	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	11
2			(p-Methoxyphenyl)-acetonil-dimet...	222	C12H18O2Si	055909-55-2	11
3			4-Aminophenyl thiocyanate, N-TMS	222	C10H14N2SSi	1000472-70-9	11
4			Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	10
5			1-((1-Butyl-1H-tetrazol-5-yl)(ph...	422	C24H31FN6	1000483-68-9	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072523\
Data File : BF134473.D
Acq On : 25 Jul 2023 20:50
Operator : CG\JU
Sample : 03647-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.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
Butane, 2-metho...	2.181	11.5	ng	371834	1	6.833	648590	20.0
n-Hexadecanoic ...	11.892	7.0	ng	184725	4	11.363	528536	20.0
1-Docosene	13.874	12.2	ng	309619	5	14.027	508194	20.0
Pentacosane	14.486	11.7	ng	297373	5	14.027	508194	20.0
Pentafluoroprop...	14.521	6.6	ng	168582	5	14.027	508194	20.0
Hexadecane	14.798	2.5	ng	41518	6	15.527	328356	20.0
Oxirane, hexade...	14.951	7.8	ng	128799	6	15.527	328356	20.0
Octadecane	15.145	9.3	ng	152357	6	15.527	328356	20.0
unknown15.209	15.209	3.4	ng	55141	6	15.527	328356	20.0
Hexacosanal	15.756	4.4	ng	71600	6	15.527	328356	20.0
unknown15.998	15.998	2.2	ng	35757	6	15.527	328356	20.0
unknown16.127	16.127	2.1	ng	34419	6	15.527	328356	20.0
unknown18.544	18.544	2.9	ng	48250	6	15.527	328356	20.0