

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
 Data File : BF130562.D
 Acq On : 06 Oct 2022 21:32
 Operator : CG\JU
 Sample : N5014-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-0-2.0

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.787	455	459	475	rVB	371091	436948	29.94%	3.728%
2	5.216	529	532	544	rBV	1328226	1363050	93.39%	11.629%
3	5.622	597	601	606	rBV	27422	23819	1.63%	0.203%
4	6.257	706	709	727	rBV	1297302	1272983	87.22%	10.861%
5	6.616	767	770	778	rBV	543522	420482	28.81%	3.587%
6	7.181	862	866	870	rBV	923521	827963	56.73%	7.064%
7	7.898	984	988	991	rBV	625340	474193	32.49%	4.046%
8	8.975	1167	1171	1174	rBV	1795783	1352154	92.64%	11.536%
9	9.645	1282	1285	1289	rBV	561267	423089	28.99%	3.610%
10	10.433	1415	1419	1430	rBV	875620	718606	49.24%	6.131%
11	11.127	1533	1537	1540	rBV	474509	406214	27.83%	3.466%
12	11.633	1619	1623	1625	rBV2	17133	18524	1.27%	0.158%
13	11.669	1625	1629	1633	rVV2	53823	56958	3.90%	0.486%
14	12.333	1739	1742	1747	rBV	108679	89059	6.10%	0.760%
15	12.563	1775	1781	1784	rBV	85656	92055	6.31%	0.785%
16	12.710	1802	1806	1810	rVB	1698287	1459531	100.00%	12.452%
17	12.992	1851	1854	1857	rBV2	17260	17897	1.23%	0.153%
18	13.504	1938	1941	1944	rBV2	15536	20318	1.39%	0.173%
19	13.610	1956	1959	1963	rBV2	15429	22593	1.55%	0.193%
20	13.757	1977	1984	1987	rBV	667465	675297	46.27%	5.761%
21	14.239	2063	2066	2069	rVB3	26758	21534	1.48%	0.184%
22	14.433	2095	2099	2111	rBV	128858	256934	17.60%	2.192%
23	14.598	2125	2127	2131	rBV4	23432	24283	1.66%	0.207%
24	14.662	2135	2138	2144	rBV	71128	79933	5.48%	0.682%
25	14.757	2150	2154	2161	rBV	104333	175051	11.99%	1.493%
26	14.833	2164	2167	2173	rVB2	80281	104079	7.13%	0.888%
27	15.027	2197	2200	2205	rVB	55408	71942	4.93%	0.614%
28	15.086	2206	2210	2215	rVB	60945	77541	5.31%	0.662%
29	15.139	2215	2219	2223	rBV	414248	462272	31.67%	3.944%
30	15.351	2253	2255	2260	rVB4	40160	50893	3.49%	0.434%
31	15.557	2286	2290	2296	rBV	74746	108001	7.40%	0.921%
32	16.262	2406	2410	2418	rBV8	29282	61638	4.22%	0.526%
33	16.445	2438	2441	2448	rVB2	28855	55294	3.79%	0.472%

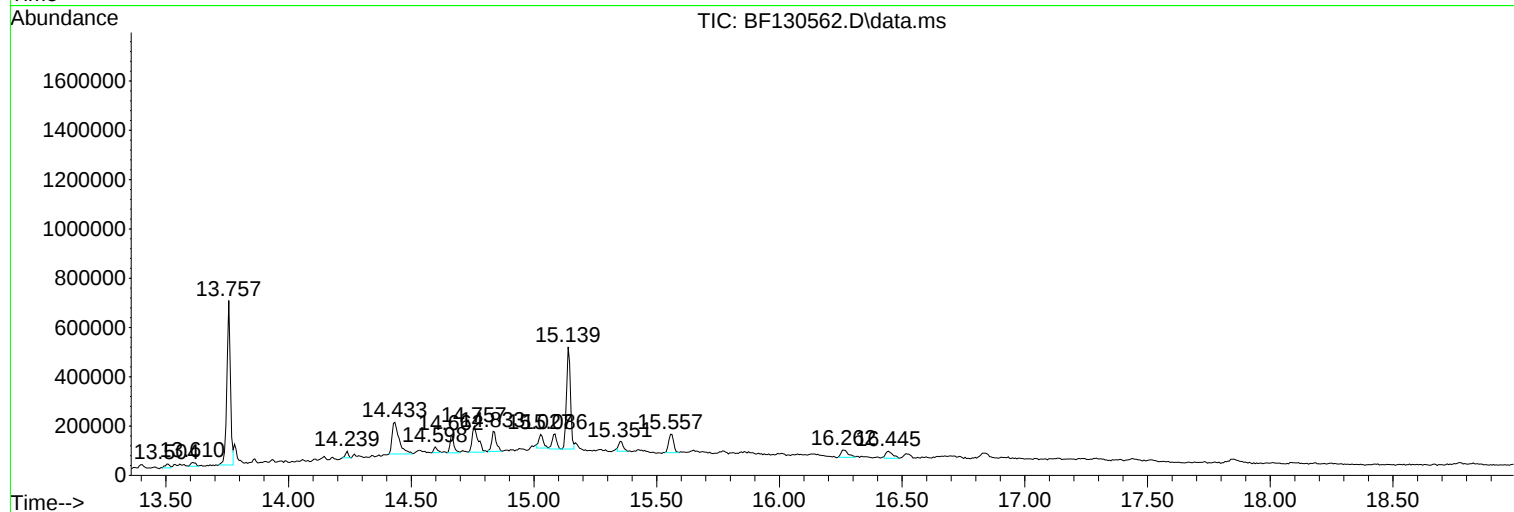
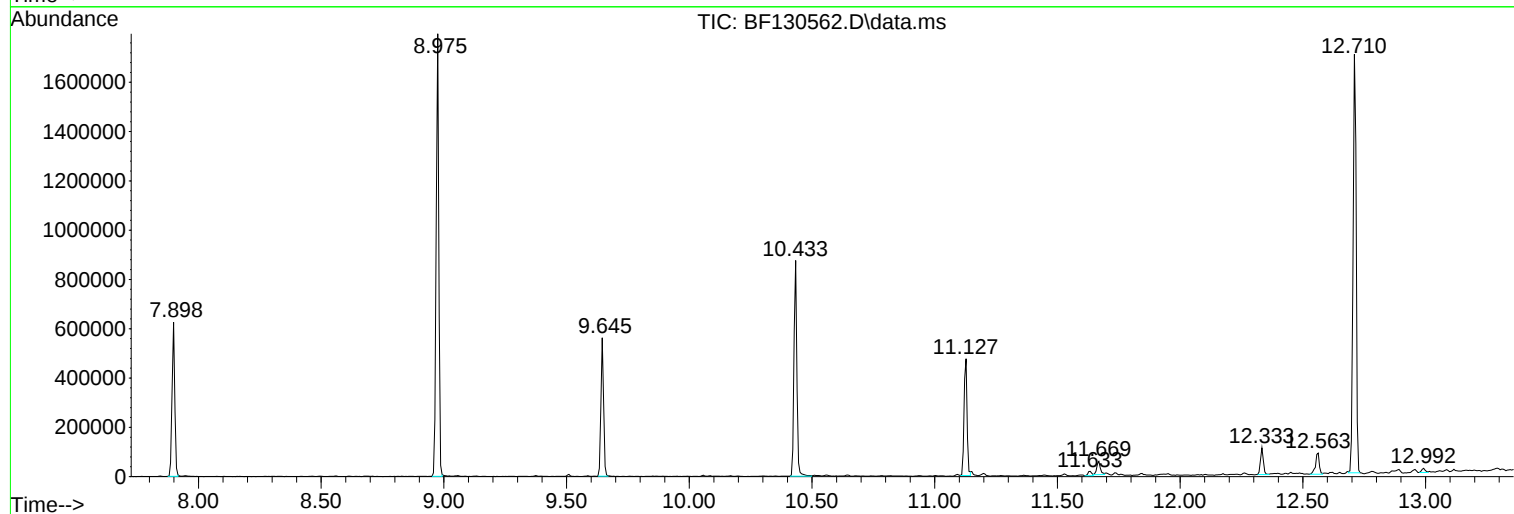
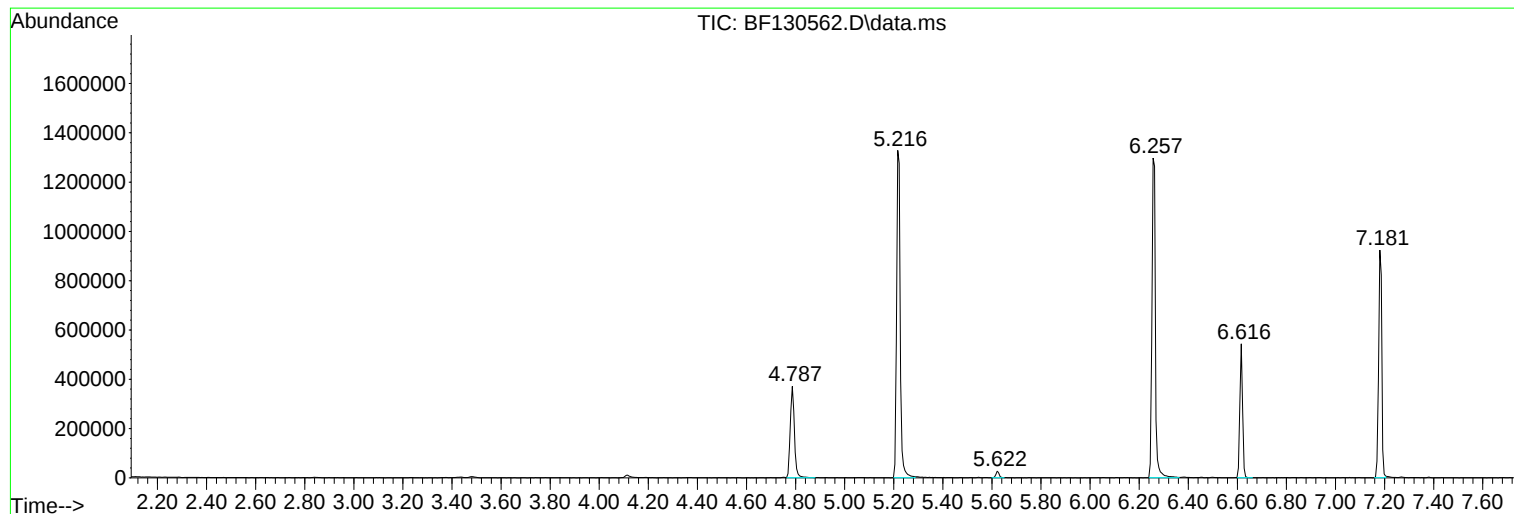
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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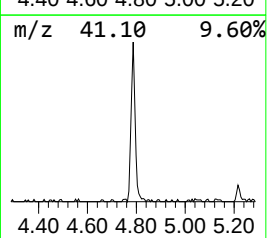
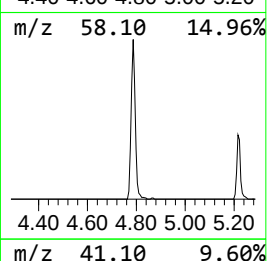
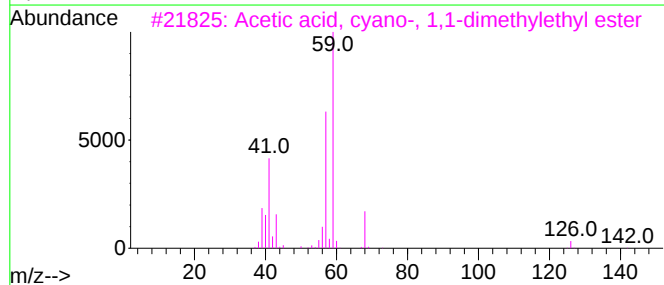
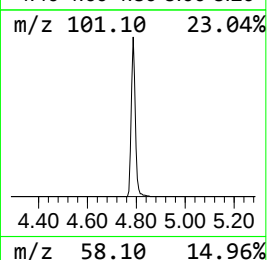
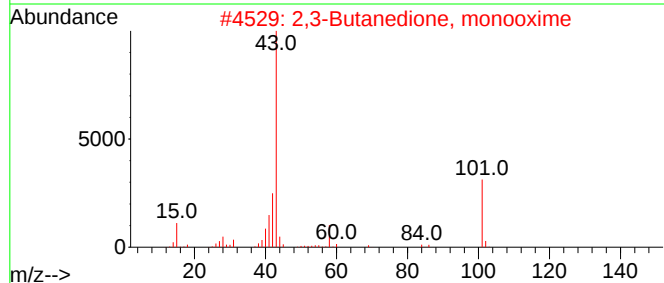
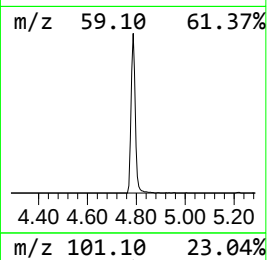
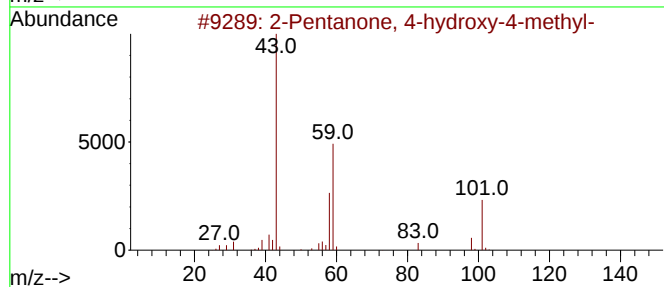
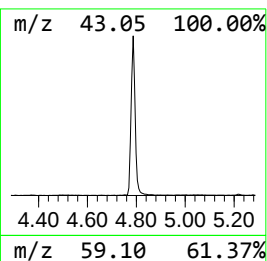
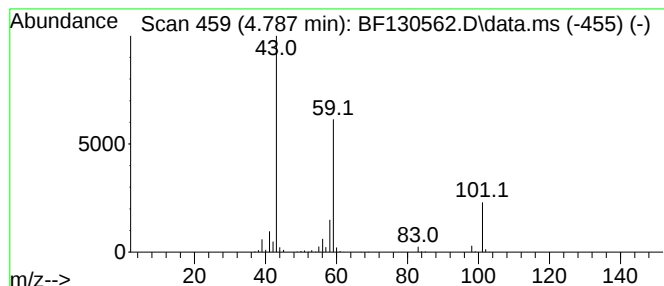
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.787	20.78 ng	436948	1,4-Dichlorobenzene-d4			6.616
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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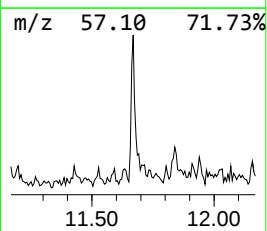
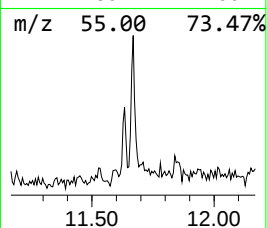
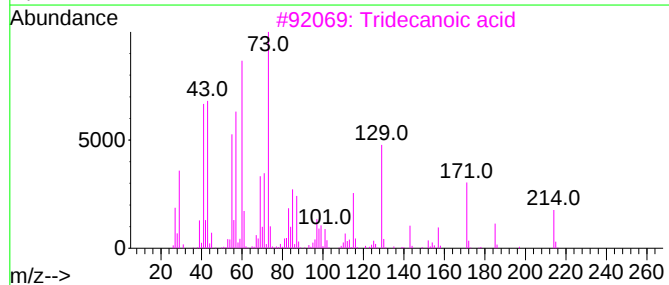
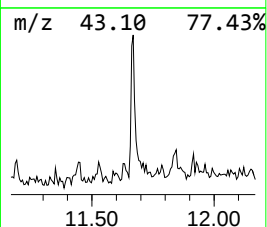
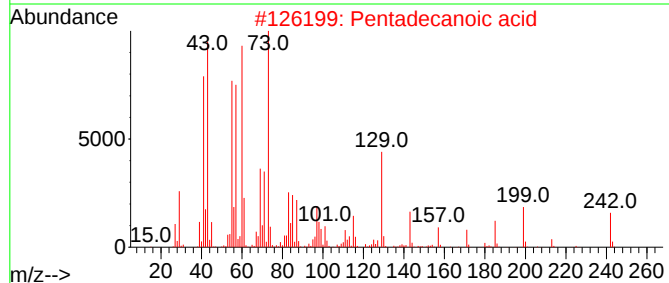
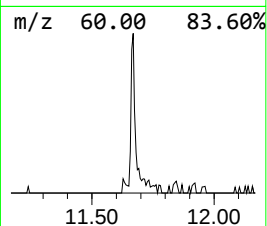
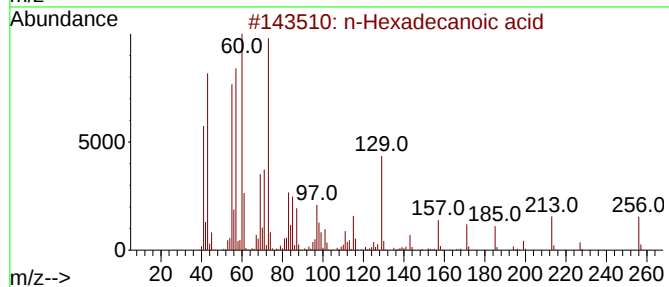
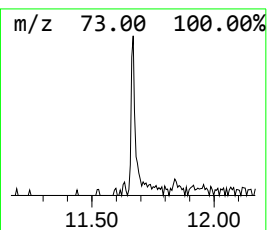
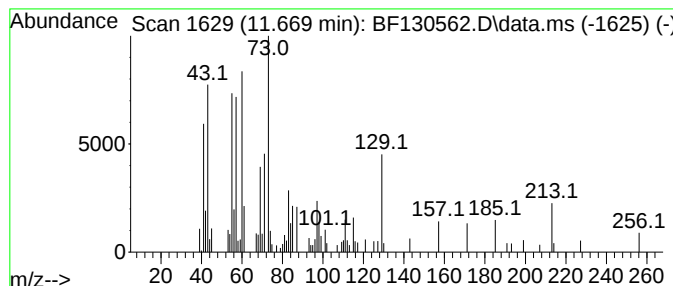
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.669	2.80 ng	56958	Phenanthrene-d10	11.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			n-Decanoic acid	172	C10H20O2	000334-48-5	59
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50



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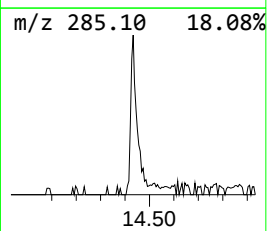
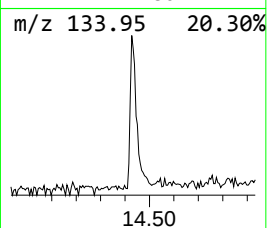
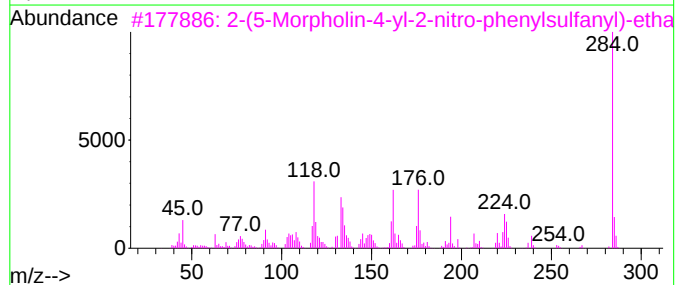
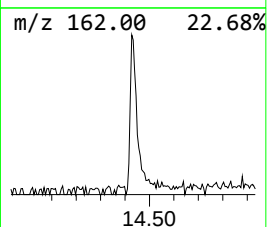
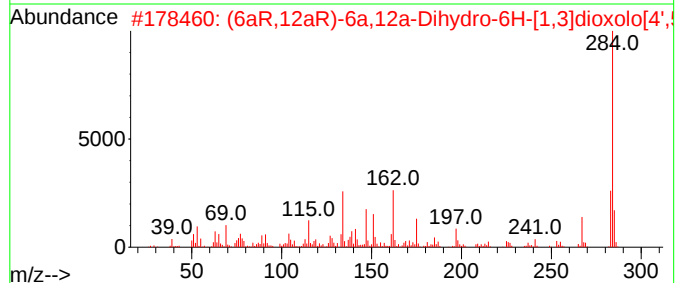
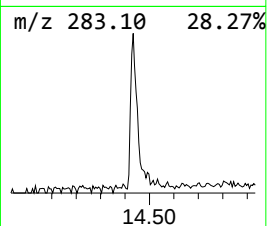
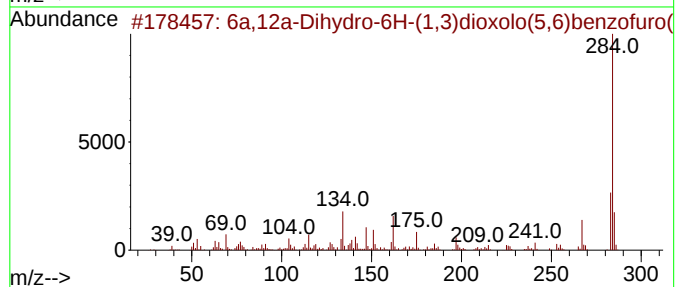
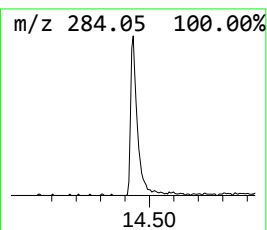
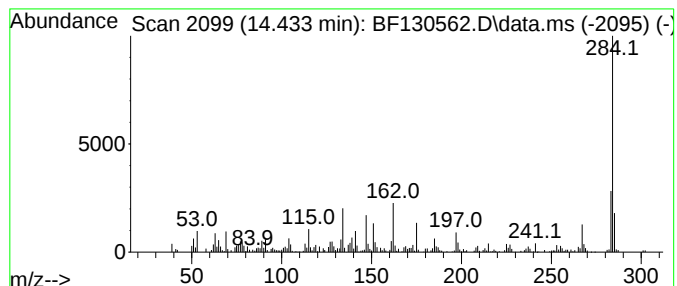
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Peak Number 3 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.433	7.61 ng	256934	Chrysene-d12	13.757	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6a,12a-Dihydro-6H-(1,3)dioxolo(5,6)benzofuro(3,4-b)pyridine	284	C16H12O5	076496-57-6	95
2	(6aR,12aR)-6a,12a-Dihydro-6H-[1,3]dioxolo[4,5-g]isoquinoline	284	C16H12O5	002035-15-6	95
3	2-(5-Morpholin-4-yl-2-nitro-phenyl)sulfanyl-ethanol	284	C12H16N2O4S	1010294-41-6	64
4	Homopterocarpin	284	C17H16O4	000606-91-7	53
5	4-Amino-5-(4-nitrophenylazo)benzofuran	284	C12H8N6O3	166766-07-0	50



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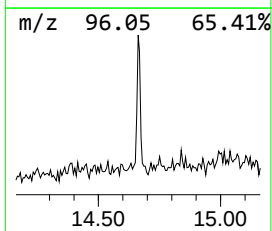
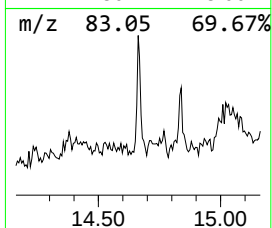
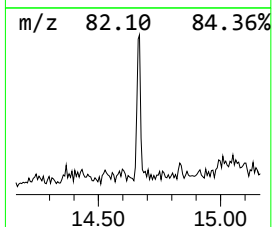
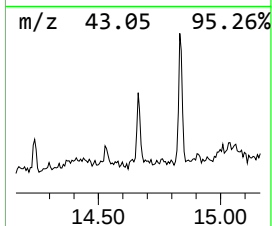
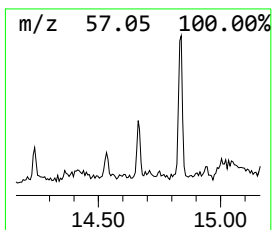
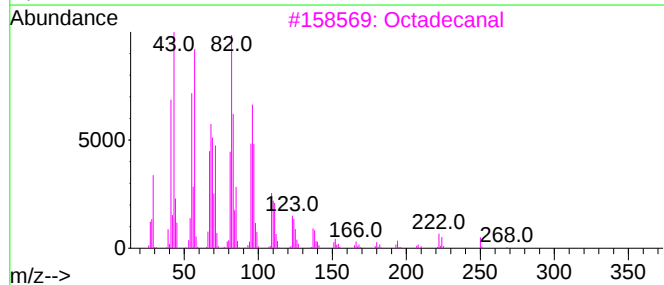
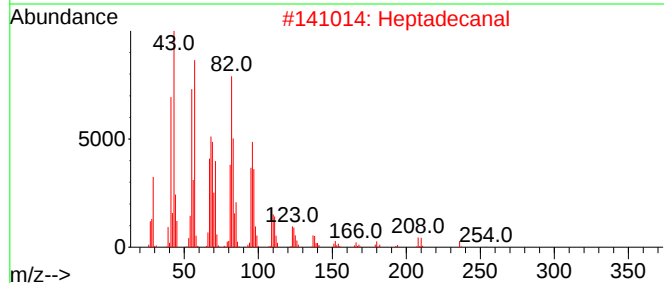
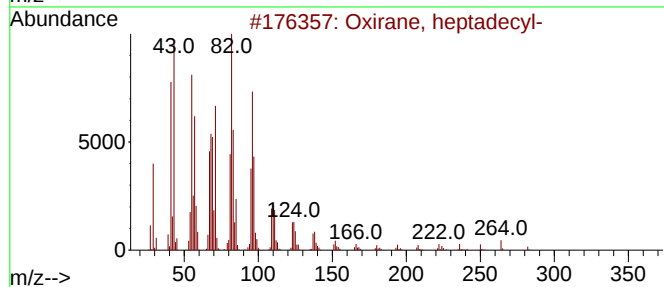
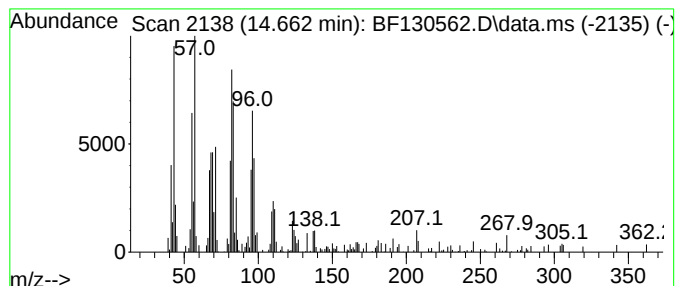
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Peak Number 4 Oxirane, heptadecyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	3.46 ng	79933	Perylene-d12	15.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2			Heptadecanal	254	C17H34O	1000376-70-0	94
3			Octadecanal	268	C18H36O	000638-66-4	91
4			Eicosanal	296	C20H40O	002400-66-0	91
5			Tetracosanal	352	C24H48O	057866-08-7	90



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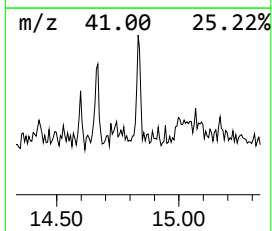
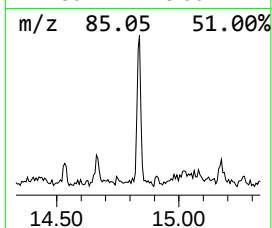
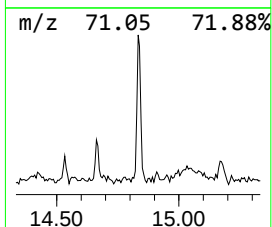
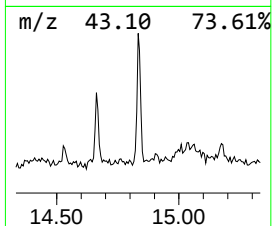
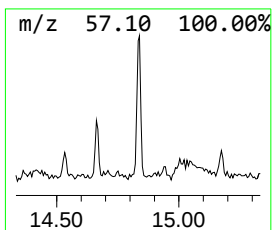
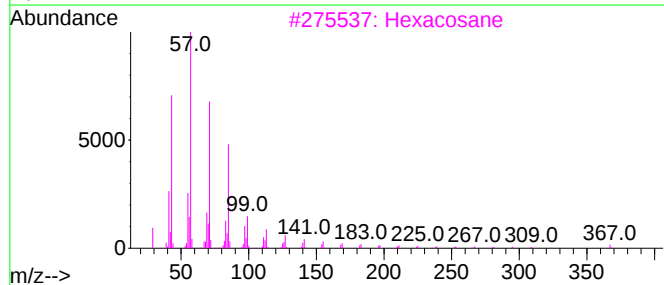
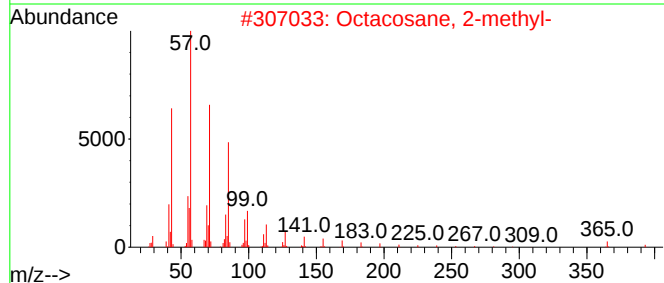
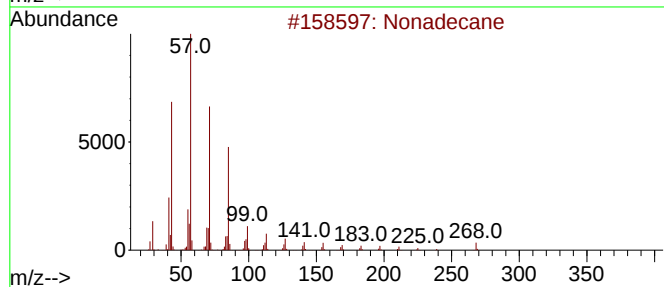
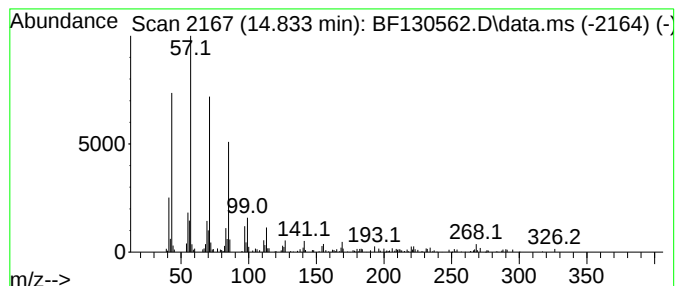
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Peak Number 5 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	4.50 ng	104079	Perylene-d12	15.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



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Sample : N5014-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-0-2.0

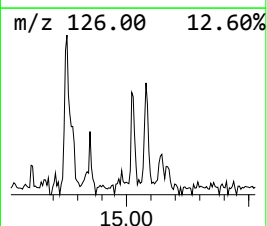
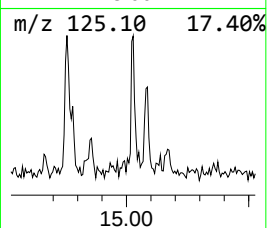
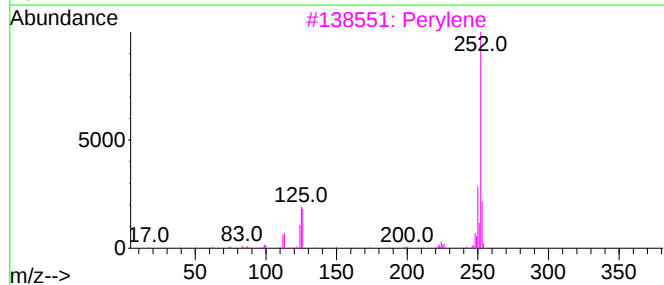
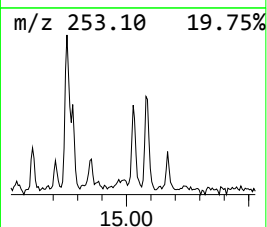
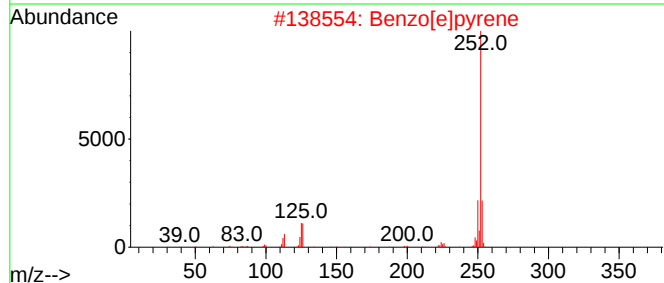
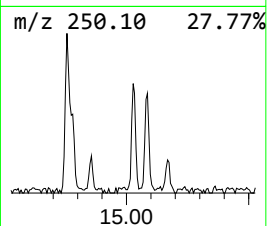
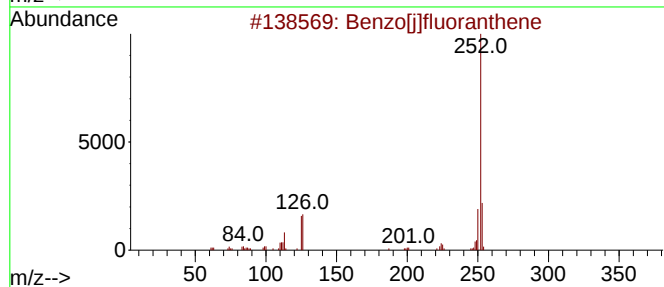
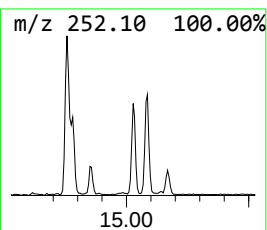
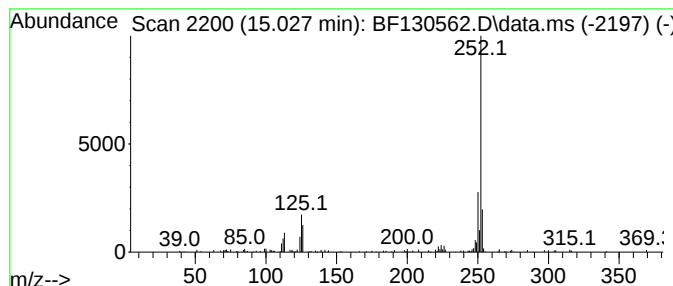
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[j]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	3.11 ng	71942	Perylene-d12	15.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	96
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130562.D
Acq On : 06 Oct 2022 21:32
Operator : CG\JU
Sample : N5014-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-0-2.0

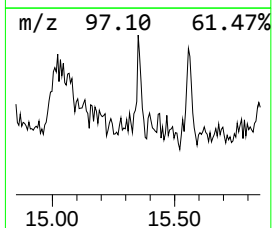
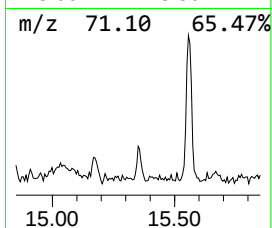
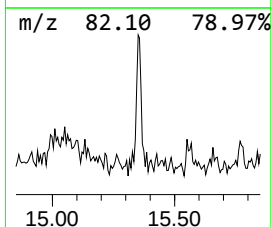
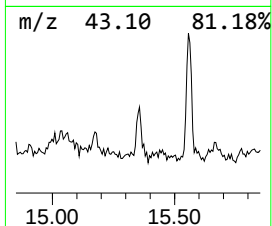
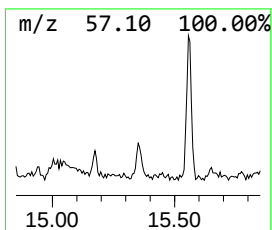
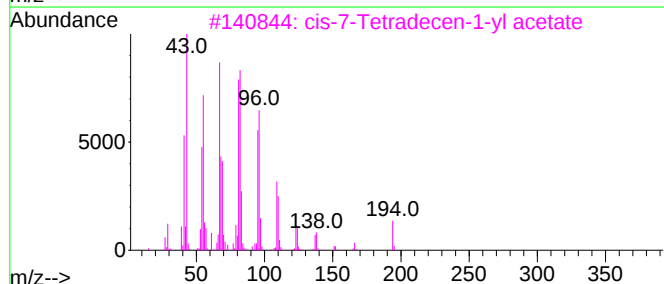
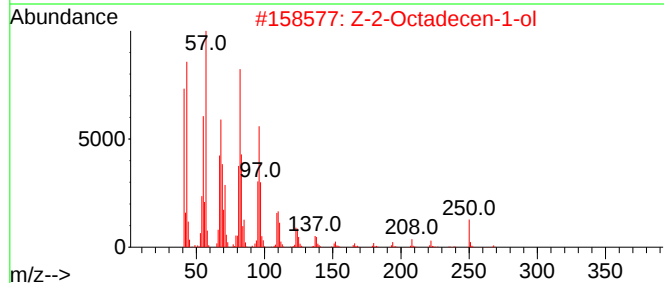
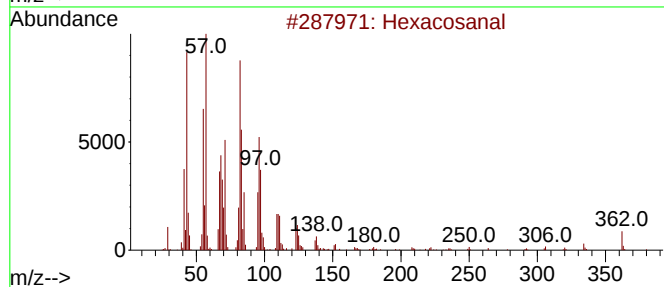
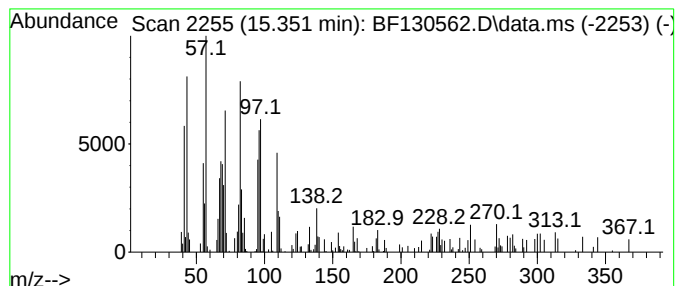
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	2.20 ng	50893	Perylene-d12	15.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosanal	380	C26H52O	026627-85-0	53
2			Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	52
3			cis-7-Tetradecen-1-yl acetate	254	C16H30O2	016974-10-0	52
4			cis-11,12-Epoxytetradecen-1-ol	270	C16H30O3	1000130-82-5	52
5			E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130562.D
Acq On : 06 Oct 2022 21:32
Operator : CG\JU
Sample : N5014-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-07-0-2.0

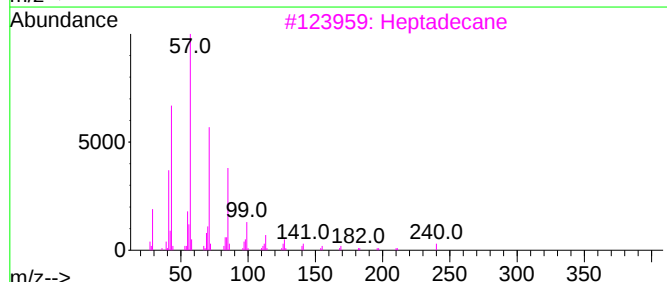
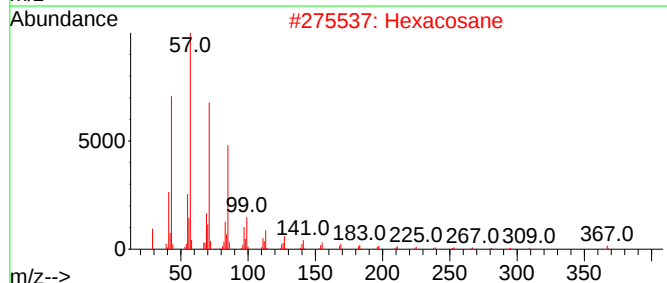
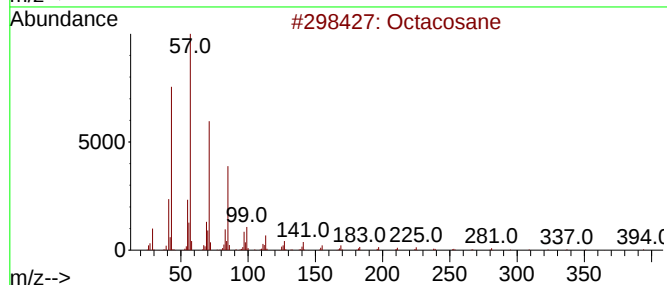
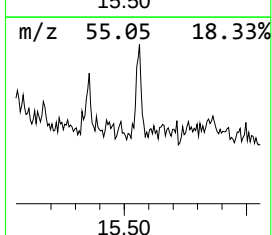
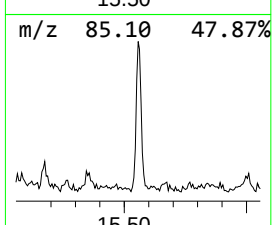
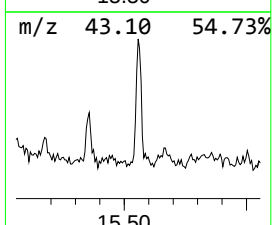
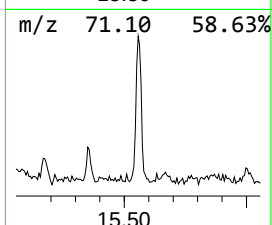
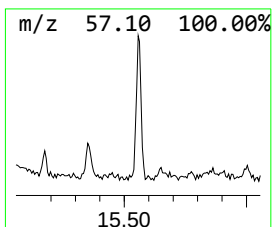
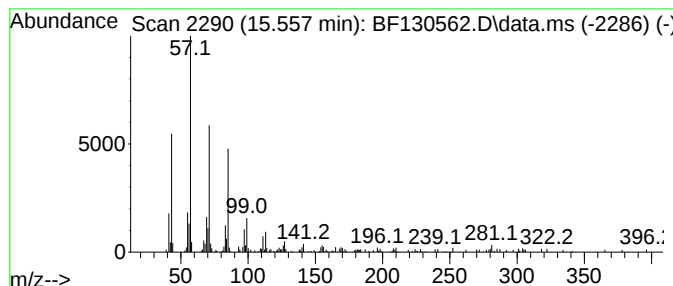
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.557	4.67 ng	108001	Perylene-d12	15.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Heptadecane	240	C17H36	000629-78-7	87
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		Tetradecane	198	C14H30	000629-59-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130562.D
Acq On : 06 Oct 2022 21:32
Operator : CG\JU
Sample : N5014-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-0-2.0

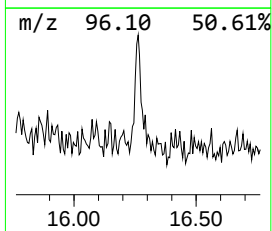
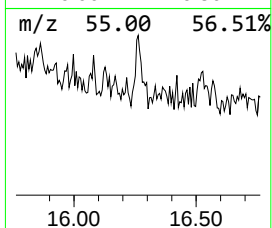
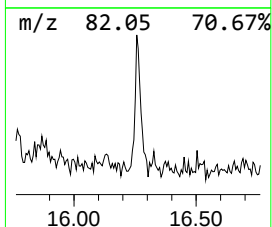
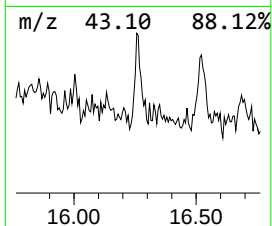
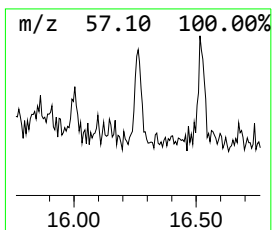
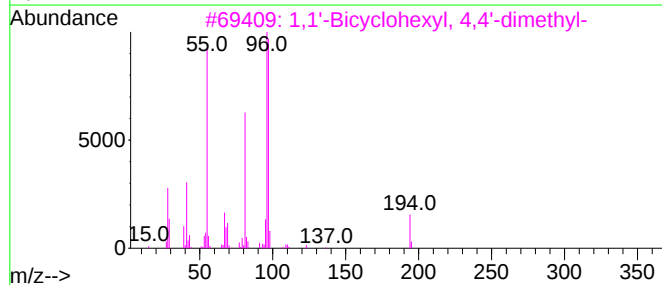
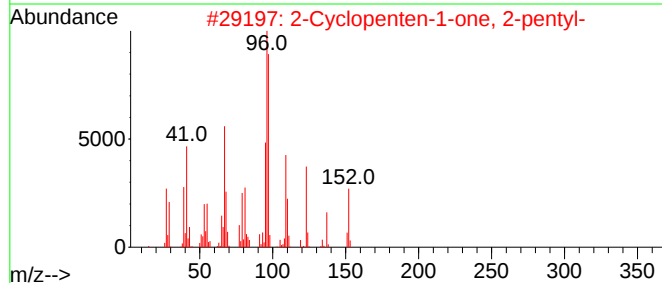
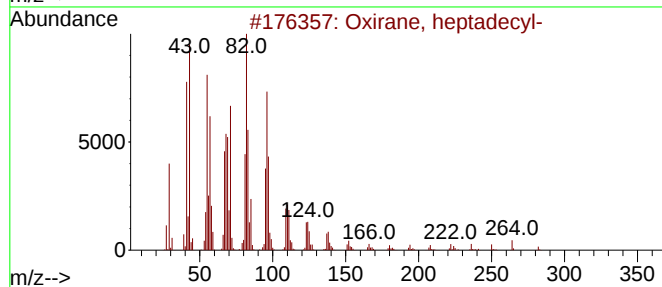
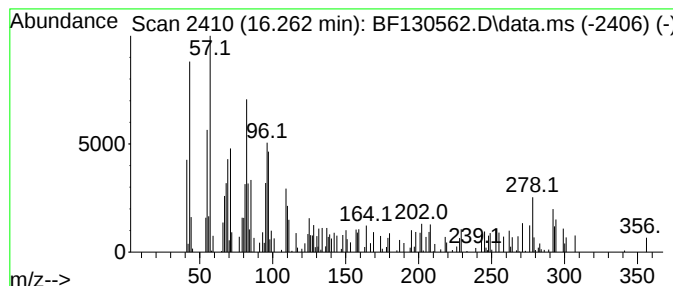
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.262 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	2.67 ng	61638	Perylene-d12	15.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	60
2			2-Cyclopenten-1-one, 2-pentyl-	152	C10H16O	025564-22-1	35
3			1,1'-Bicyclohexyl, 4,4'-dimethyl-	194	C14H26	054823-99-3	35
4			Henicosanal	310	C21H42O	051227-32-8	25
5			Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130562.D
Acq On : 06 Oct 2022 21:32
Operator : CG\JU
Sample : N5014-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

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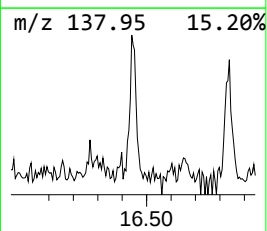
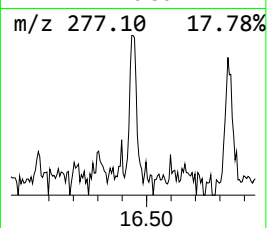
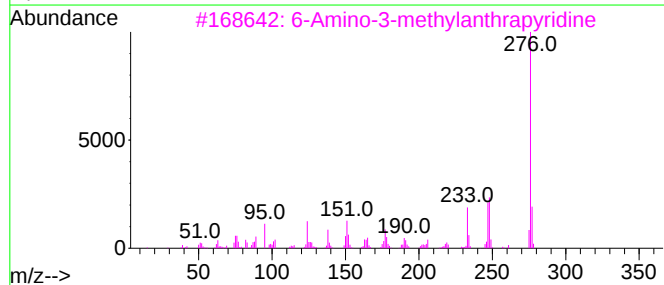
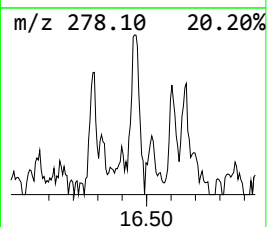
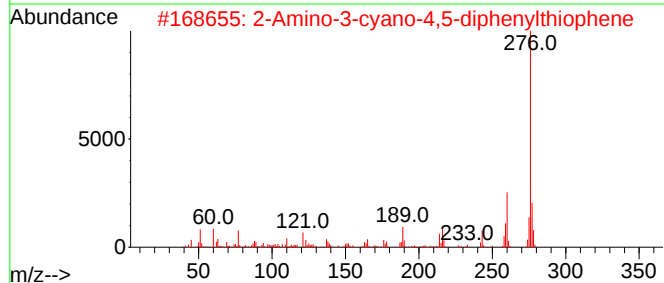
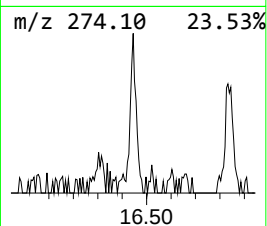
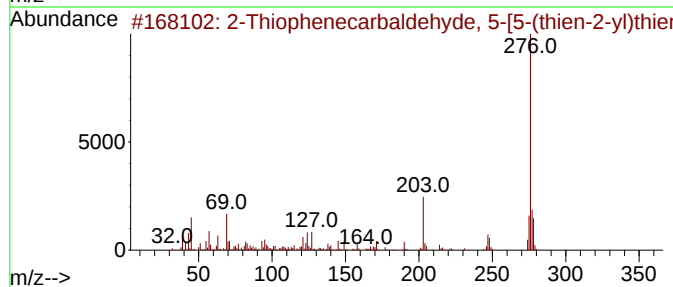
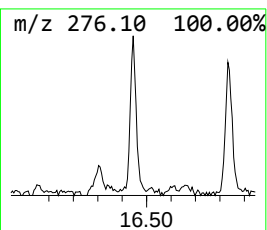
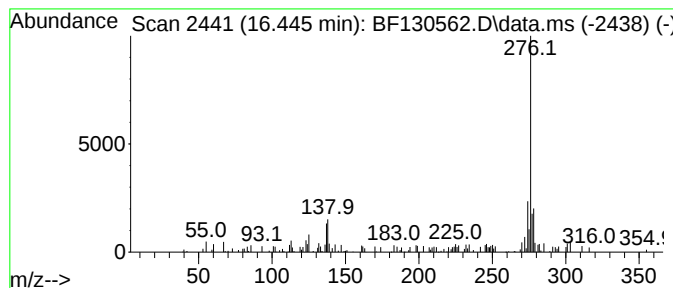
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Thiophenecarbaldehyde, 5-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	2.39 ng	55294	Perylene-d12	15.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	53
2			2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	50
3			6-Amino-3-methylantrapyridine	276	C17H12N2O2	014642-72-9	47
4			12H-Benzothieno[2,3-d]pyrido[1,2...	276	C14H16N2S2	102254-63-7	47
5			Ethyl 5-pentyl-2-thioxo-1,3-dith...	276	C11H16O2S3	120356-16-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130562.D
Acq On : 06 Oct 2022 21:32
Operator : CG\JU
Sample : N5014-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.787	20.8	ng	436948	1	6.616	420482	20.0
n-Hexadecanoic ...	11.669	2.8	ng	56958	4	11.127	406214	20.0
6a,12a-Dihydro-...	14.433	7.6	ng	256934	5	13.757	675297	20.0
Oxirane, heptad...	14.663	3.5	ng	79933	6	15.139	462272	20.0
Nonadecane	14.833	4.5	ng	104079	6	15.139	462272	20.0
Benzo[j]fluoran...	15.027	3.1	ng	71942	6	15.139	462272	20.0
Hexacosanal	15.351	2.2	ng	50893	6	15.139	462272	20.0
Octacosane	15.557	4.7	ng	108001	6	15.139	462272	20.0
unknown16.262	16.262	2.7	ng	61638	6	15.139	462272	20.0
2-Thiophenecarb...	16.445	2.4	ng	55294	6	15.139	462272	20.0