

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128543.D
 Acq On : 28 May 2022 12:33
 Operator : CG\JU
 Sample : N2928-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P026-SS001-0006-01

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: BF128543.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.934	105	110	116	rBV	41790	64822	1.78%	0.215%
2	3.904	271	275	280	rVB	29367	38491	1.06%	0.128%
3	5.051	467	470	478	rVB	69563	77058	2.12%	0.255%
4	5.445	532	537	540	rBV	2855459	2670486	73.41%	8.854%
5	6.287	676	680	694	rBV2	158730	239575	6.59%	0.794%
6	6.457	704	709	712	rBV	2885333	2805100	77.12%	9.300%
7	6.575	725	729	743	rBV2	207094	305532	8.40%	1.013%
8	6.834	770	773	777	rBV	1422536	1244424	34.21%	4.126%
9	7.398	863	869	872	rBV	2110158	1943379	53.43%	6.443%
10	8.122	987	992	995	rBV	1727804	1656294	45.53%	5.491%
11	9.198	1169	1175	1178	rBV	4029095	3637553	100.00%	12.060%
12	9.875	1283	1290	1294	rBV	2252986	1888096	51.91%	6.260%
13	10.663	1419	1424	1427	rBV	2502969	2211830	60.81%	7.333%
14	11.363	1539	1543	1546	rBV	2229833	1864926	51.27%	6.183%
15	11.892	1629	1633	1642	rBV2	471351	464473	12.77%	1.540%
16	11.980	1645	1648	1652	rVB	66219	56157	1.54%	0.186%
17	12.163	1673	1679	1686	rVB5	30441	65127	1.79%	0.216%
18	12.474	1724	1732	1733	rBV3	53762	83509	2.30%	0.277%
19	12.492	1733	1735	1738	rVB	131889	103110	2.83%	0.342%
20	12.674	1762	1766	1770	rBV2	293774	308085	8.47%	1.021%
21	12.710	1770	1772	1777	rVB	59203	57565	1.58%	0.191%
22	12.839	1790	1794	1799	rVB4	44673	45889	1.26%	0.152%
23	12.892	1800	1803	1805	rVB	67863	52068	1.43%	0.173%
24	12.951	1809	1813	1818	rVB	3679739	3294686	90.57%	10.923%
25	13.133	1841	1844	1847	rVB	109309	98390	2.70%	0.326%
26	13.168	1847	1850	1852	rBV	137436	112499	3.09%	0.373%
27	13.321	1873	1876	1879	rVB	114154	98349	2.70%	0.326%
28	13.357	1879	1882	1884	rBV2	64137	60717	1.67%	0.201%
29	13.427	1891	1894	1899	rVB	111107	95700	2.63%	0.317%
30	13.539	1908	1913	1917	rBV2	146301	183465	5.04%	0.608%
31	13.898	1970	1974	1987	rVB4	170397	381042	10.48%	1.263%
32	13.998	1987	1991	1995	rBV	1305650	1259647	34.63%	4.176%
33	14.098	2003	2008	2017	rVB	409152	473786	13.02%	1.571%
34	14.480	2070	2073	2077	rBV	80541	75244	2.07%	0.249%
35	15.098	2174	2178	2180	rBV	104285	116722	3.21%	0.387%
36	15.133	2180	2184	2190	rVB	141692	177987	4.89%	0.590%

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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

37	15.468	2235	2241	2245	rBV	774174	984153	27.06%	3.263%
38	15.951	2319	2323	2331	rVB	97558	140910	3.87%	0.467%
39	16.092	2340	2347	2360	rBV6	96962	352492	9.69%	1.169%
40	16.751	2454	2459	2466	rVB	168119	303340	8.34%	1.006%
41	17.609	2600	2605	2606	rBV4	47266	69395	1.91%	0.230%

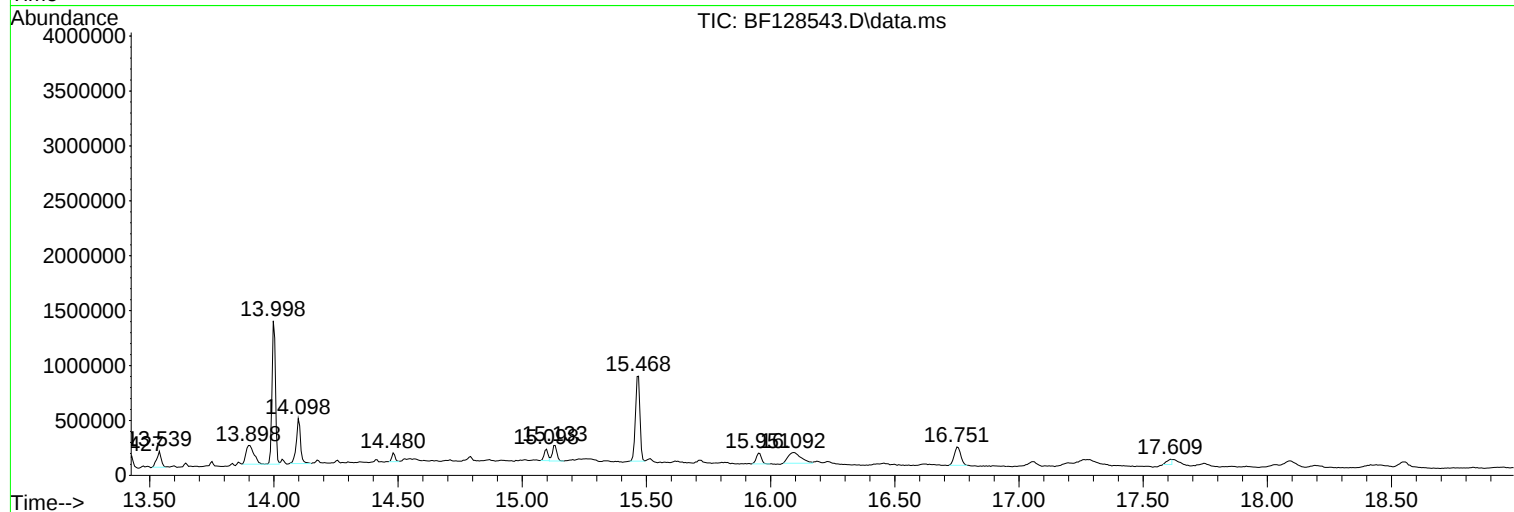
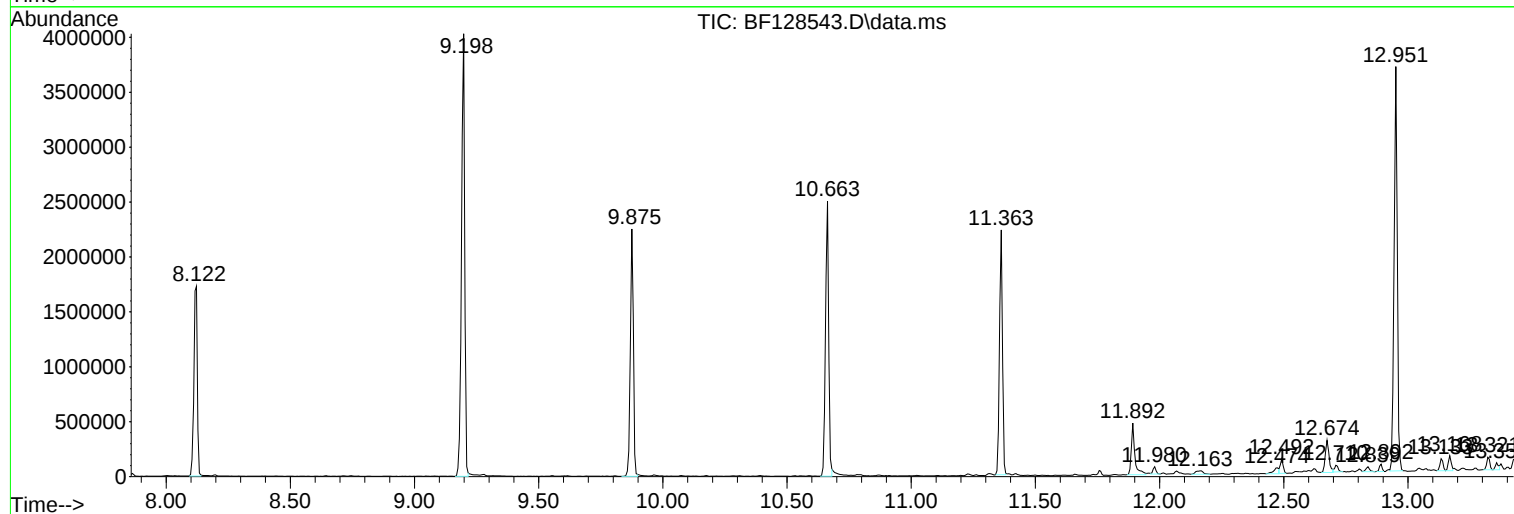
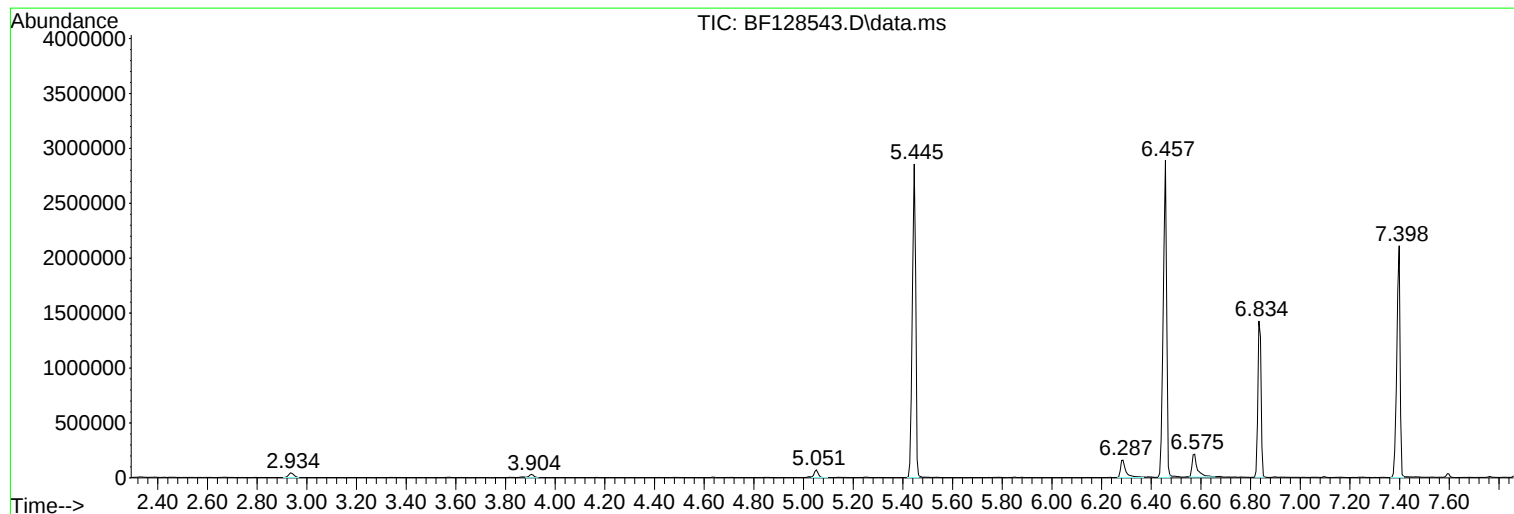
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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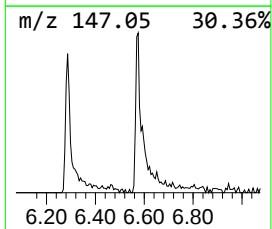
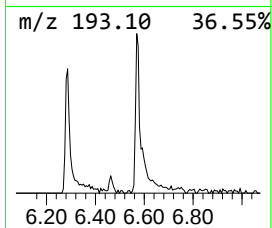
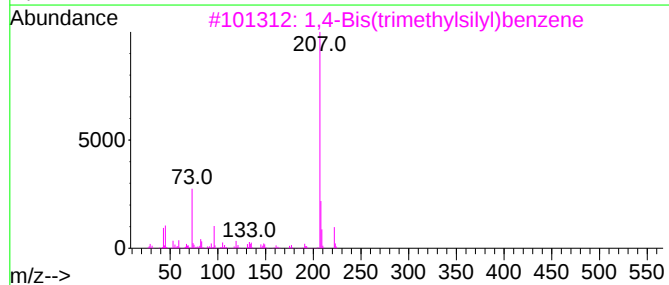
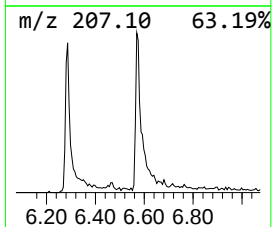
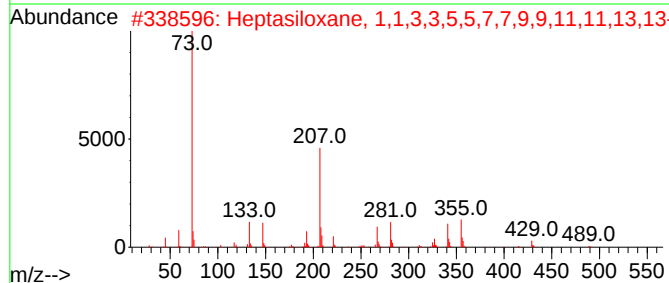
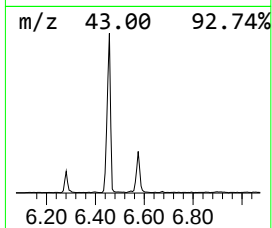
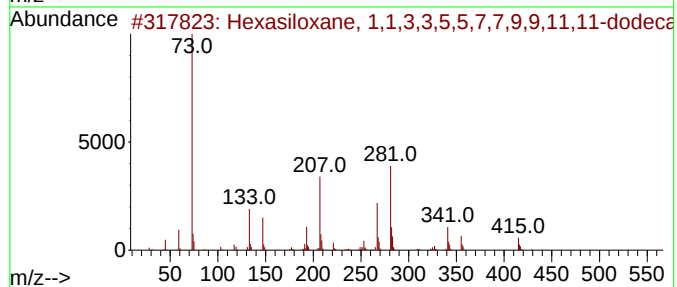
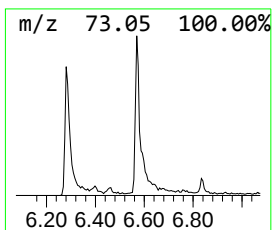
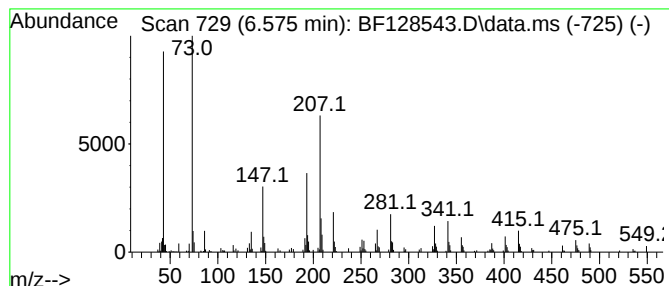
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.575 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.575	4.91 ng	305532	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	43
2			Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	32
3			1,4-Bis(trimethylsilyl)benzene	222	C12H22Si2	013183-70-5	30
4			1,2-Bis(trimethylsilyl)benzene	222	C12H22Si2	017151-09-6	30
5			N-(2-Hydroxyethyl)-N'-(2-methoxy...	354	C16H30N2O3Si2	1000501-33-3	27



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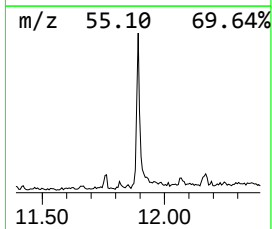
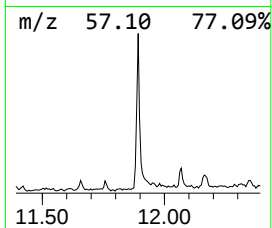
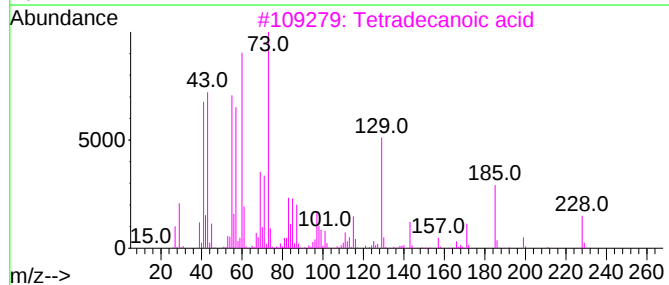
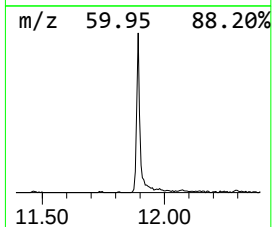
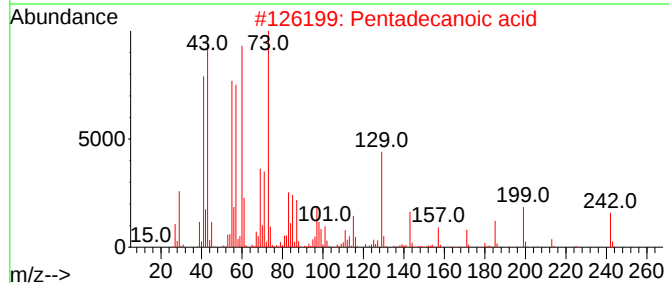
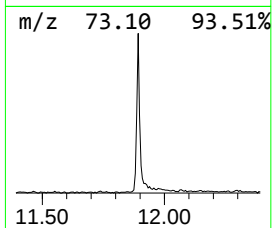
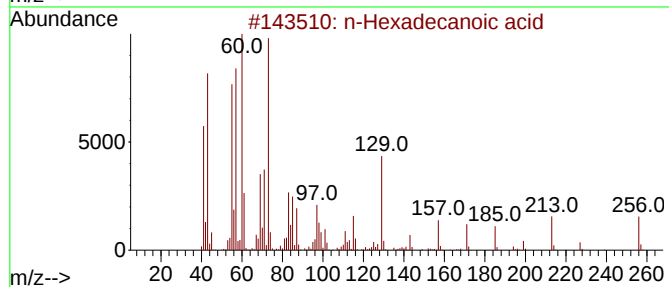
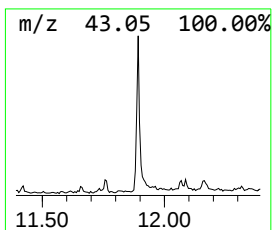
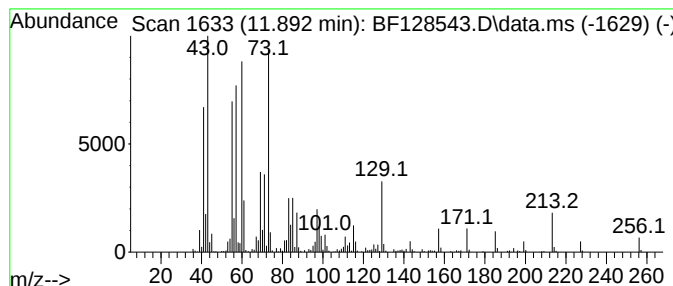
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.98 ng	464473	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Nonanoic acid	158	C9H18O2	000112-05-0	53



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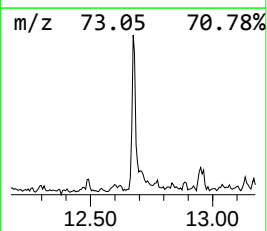
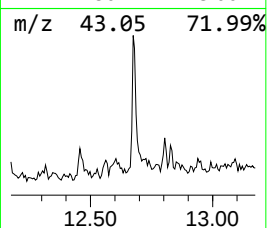
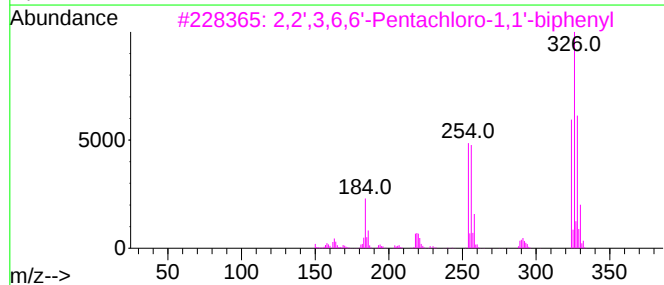
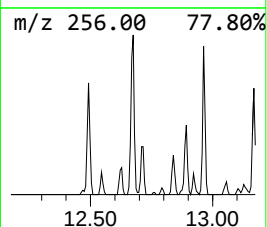
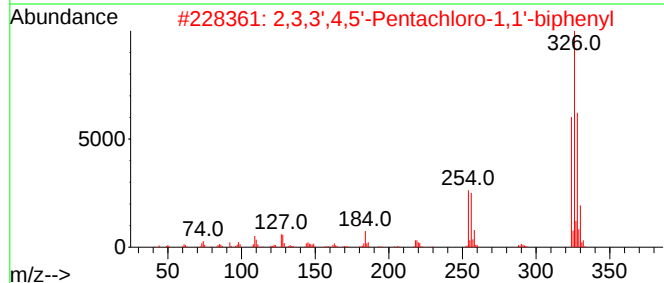
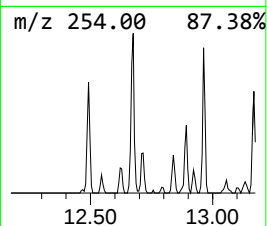
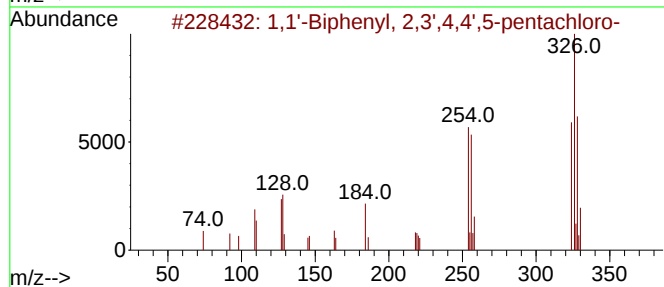
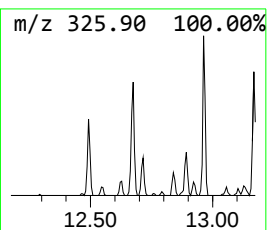
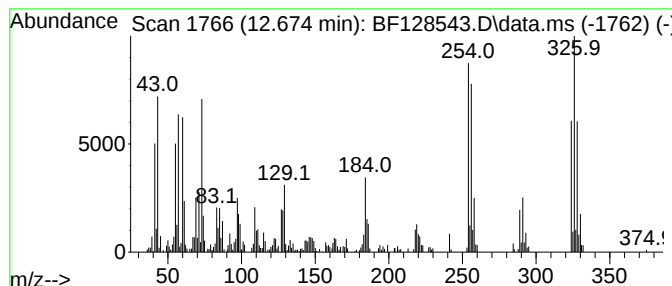
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1'-Biphenyl, 2,3',4,4',5-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.674	3.30 ng	308085	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,3',4,4',5-penta...	324	C12H5Cl5	031508-00-6	99
2	2,3,3',4,5'-Pentachloro-1,1'-bip...	324	C12H5Cl5	070362-41-3	99
3	2,2',3,6,6'-Pentachloro-1,1'-bip...	324	C12H5Cl5	073575-54-9	99
4	2,3,3',4,5-Pentachloro-1,1'-biph...	324	C12H5Cl5	070424-69-0	99
5	2,3,3',4',5'- Pentachloro-1,1'-b...	324	C12H5Cl5	076842-07-4	99



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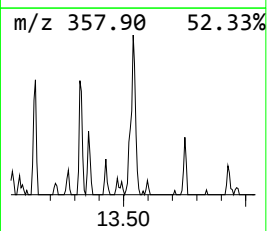
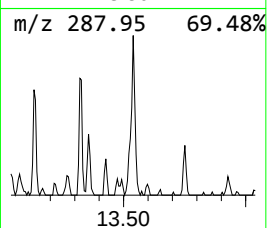
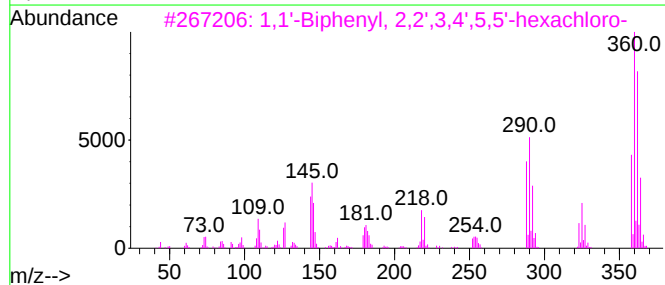
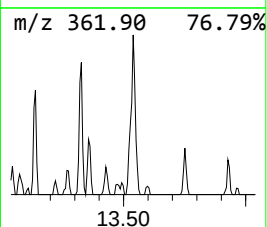
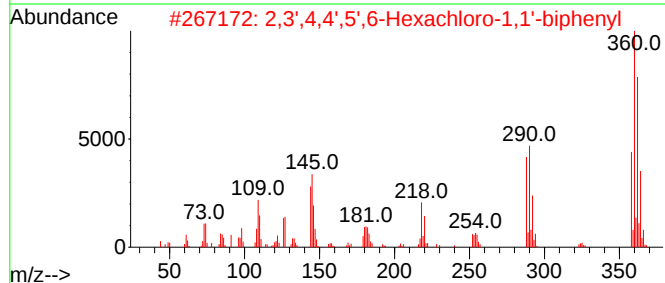
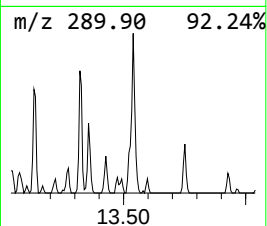
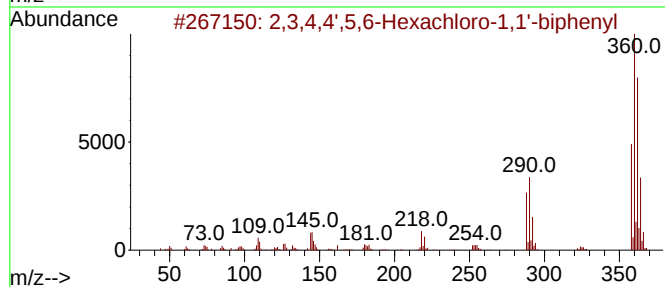
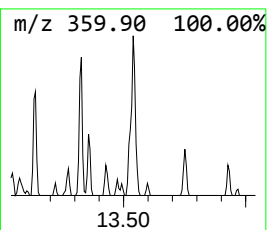
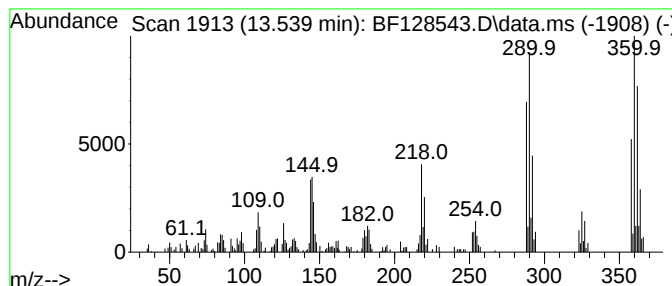
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2,3,4,4',5,6-Hexachloro-1,1... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.539	2.91 ng	183465	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,4,4',5,6-Hexachloro-1,1'-bip...	358	C12H4Cl6	041411-63-6	99		
2	2,3',4,4',5',6-Hexachloro-1,1'-b...	358	C12H4Cl6	059291-65-5	99		
3	1,1'-Biphenyl, 2,2',3,4',5,5'-he...	358	C12H4Cl6	051908-16-8	99		
4	2,3,3',4,5,5'-Hexachloro-1,1'-bi...	358	C12H4Cl6	039635-35-3	99		
5	1,1'-Biphenyl, 2,3,3',4,4',5'-he...	358	C12H4Cl6	069782-90-7	99		



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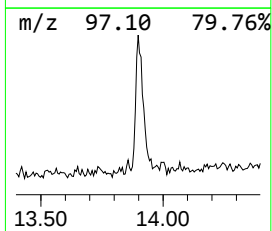
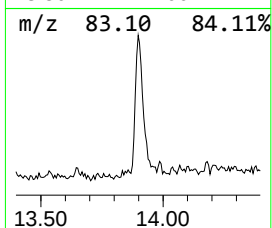
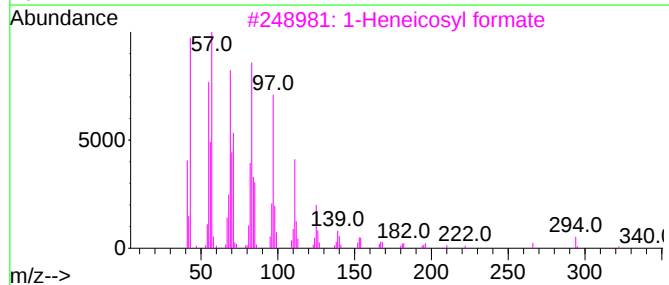
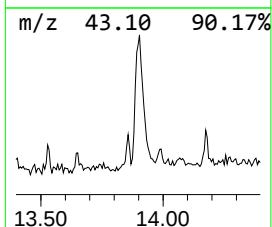
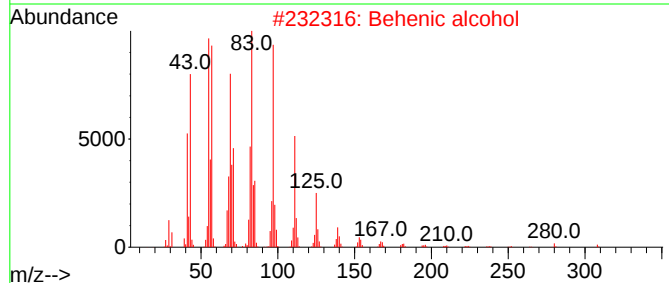
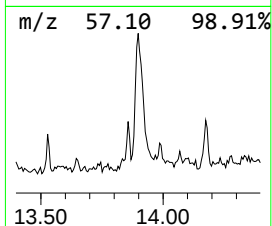
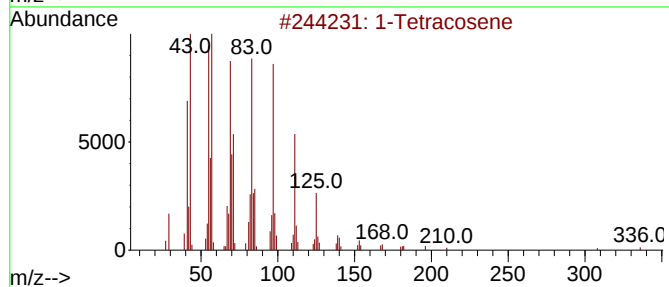
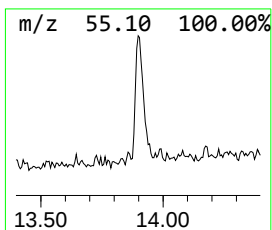
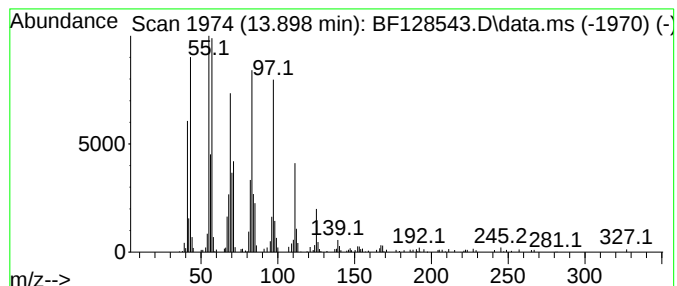
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tetracosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	6.05 ng	381042	Chrysene-d12	13.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128543.D
Acq On : 28 May 2022 12:33
Operator : CG\JU
Sample : N2928-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P026-SS001-0006-01

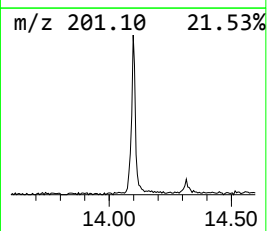
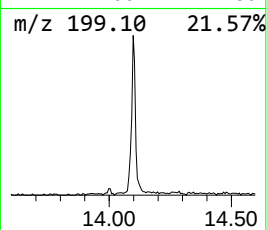
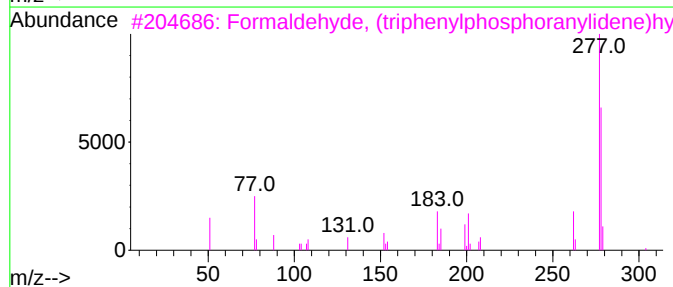
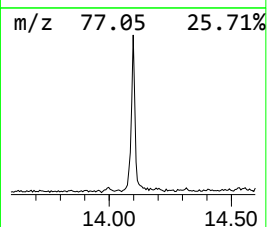
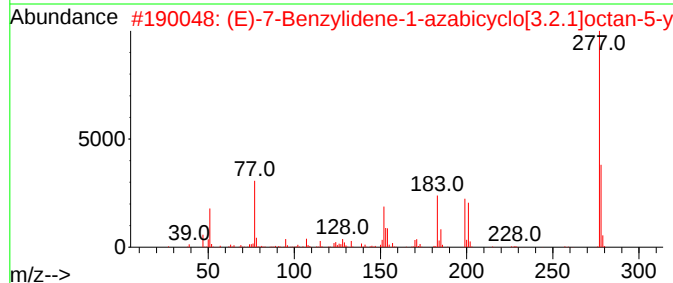
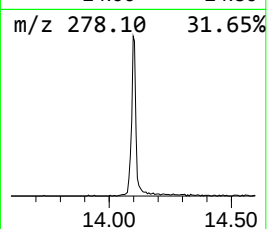
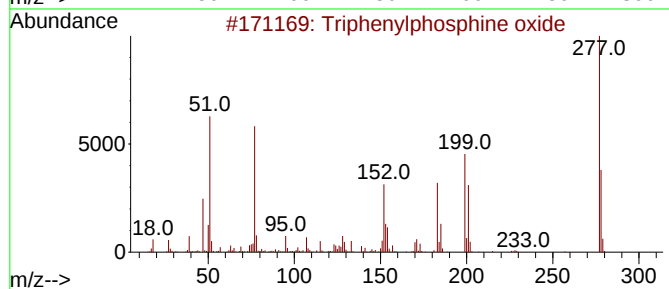
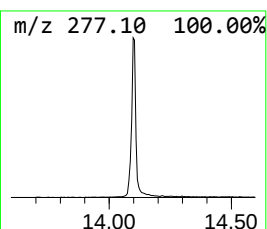
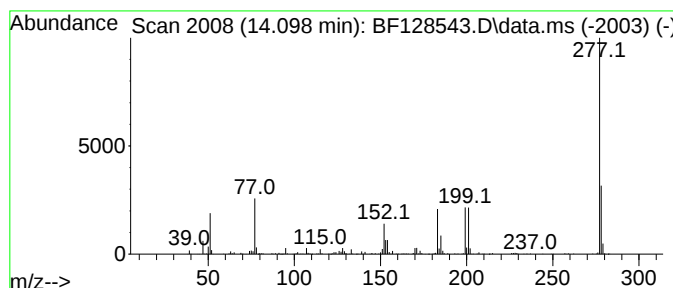
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	7.52 ng	473786	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	94
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
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Acq On : 28 May 2022 12:33
Operator : CG\JU
Sample : N2928-04
Misc :
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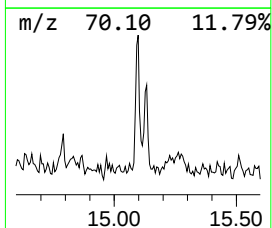
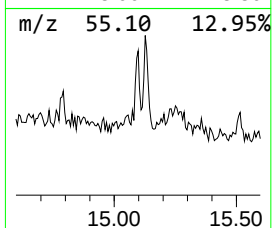
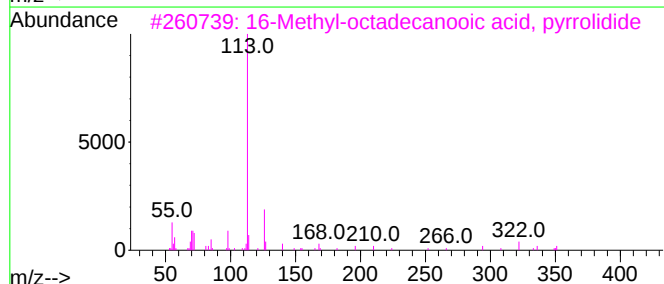
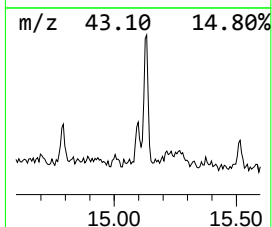
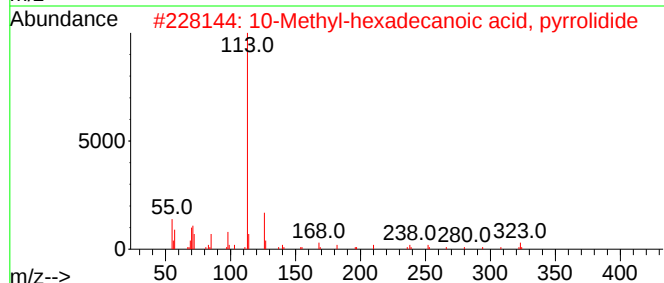
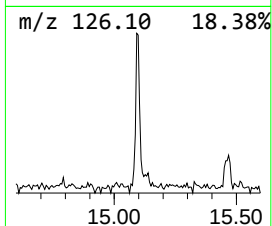
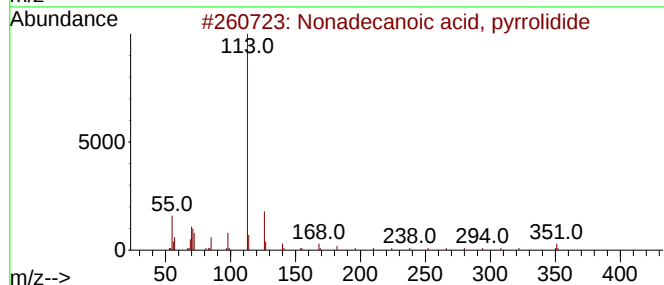
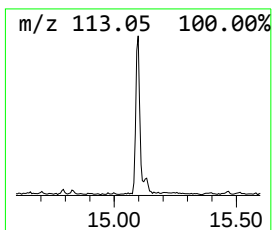
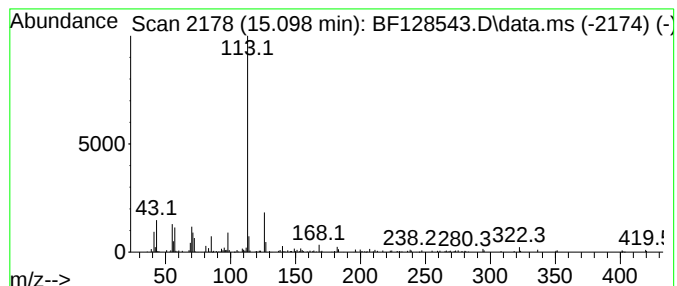
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecanoic acid, pyrrolidide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.098	2.37 ng	116722	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecanoic acid, pyrrolidide	351	C23H45NO	1000336-08-0	95
2	10-Methyl-hexadecanoic acid, pyr...	323	C21H41NO	1000336-18-3	95
3	16-Methyl-octadecanoic acid, py...	351	C23H45NO	1000336-03-8	93
4	11-Methyl-octadecanoic acid, pyr...	351	C23H45NO	959259-82-6	87
5	Pyrrolidine, 1-(6-methyl-1-oxooc...	351	C23H45NO	056600-07-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128543.D
Acq On : 28 May 2022 12:33
Operator : CG\JU
Sample : N2928-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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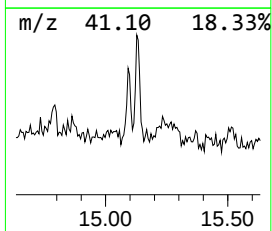
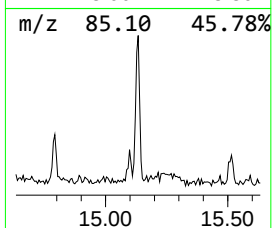
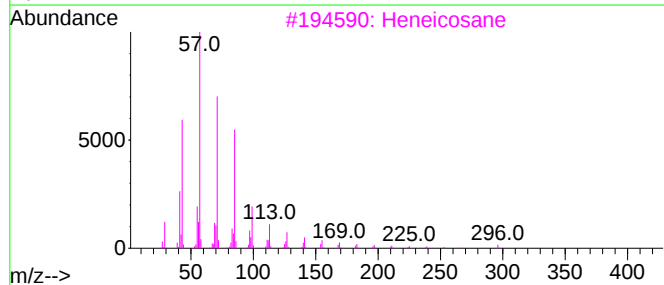
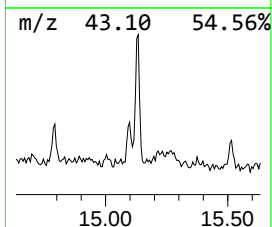
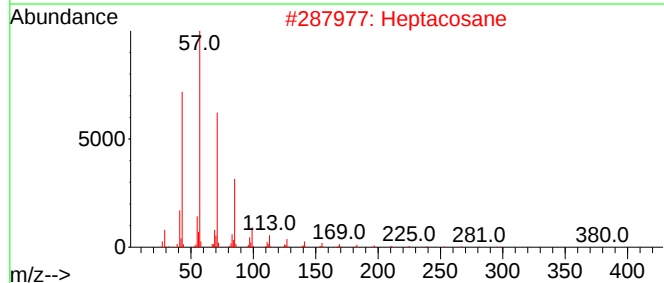
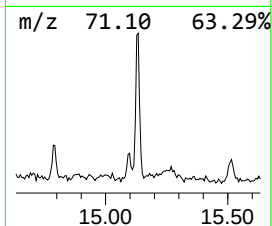
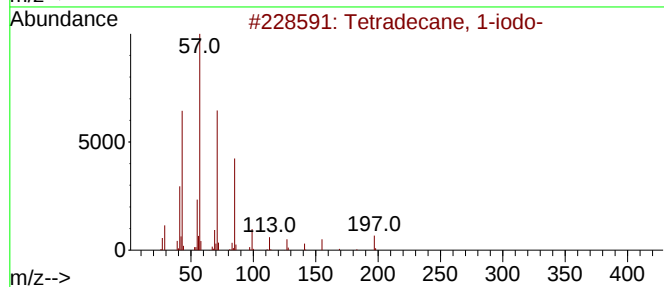
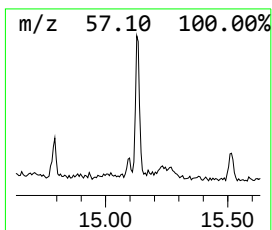
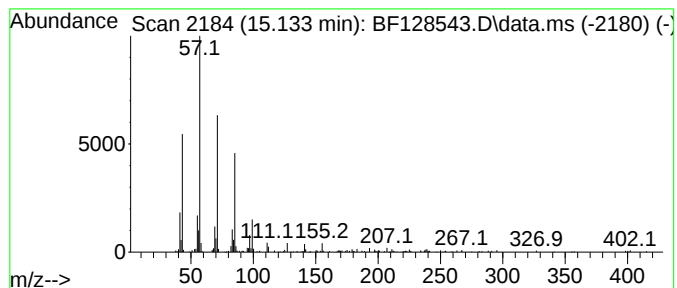
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	3.62 ng	177987	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
2			Heptacosane	380	C27H56	000593-49-7	86
3			Heneicosane	296	C21H44	000629-94-7	80
4			Undecane, 3-methyl-	170	C12H26	001002-43-3	80
5			Pentadecane, 3-methyl-	226	C16H34	002882-96-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
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Acq On : 28 May 2022 12:33
Operator : CG\JU
Sample : N2928-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

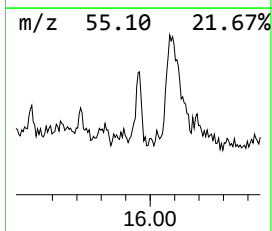
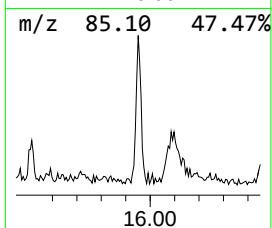
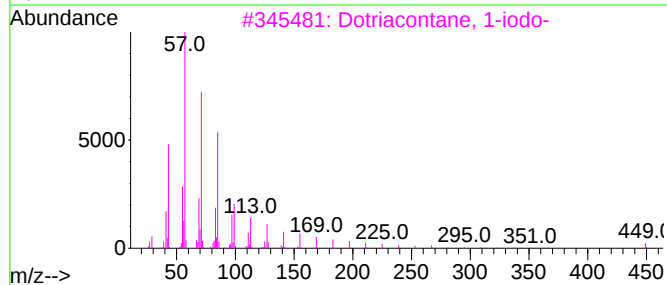
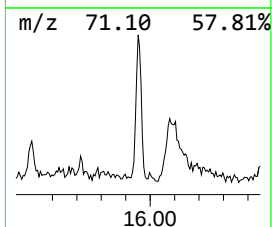
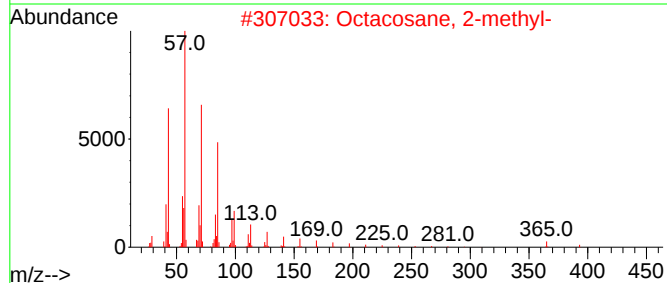
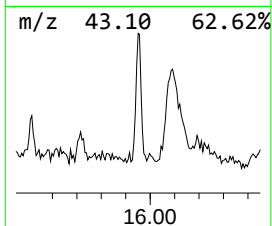
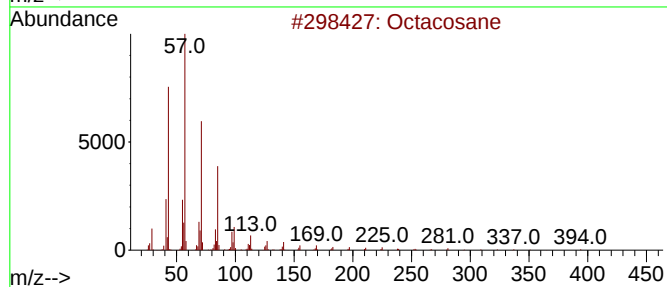
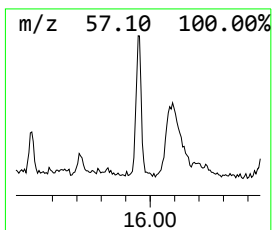
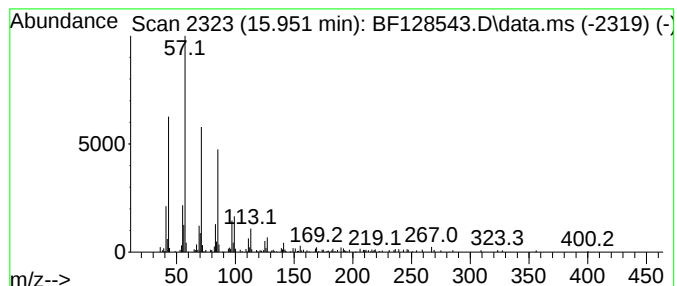
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.951	2.86 ng	140910	Perylene-d12		15.468	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	Octacosane, 2-methyl-		408	C29H60	001560-98-1	87
3	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	87
4	Hexacosane		366	C26H54	000630-01-3	87
5	Eicosane		282	C20H42	000112-95-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
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Sample : N2928-04
Misc :
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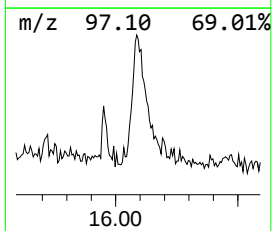
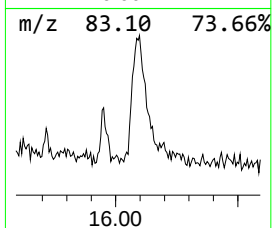
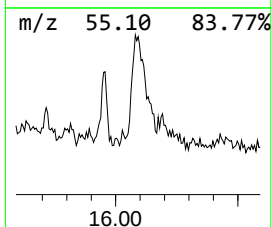
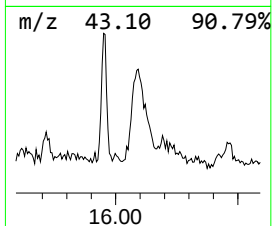
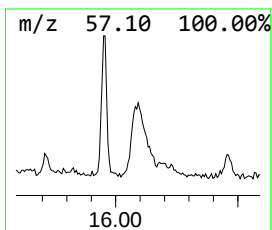
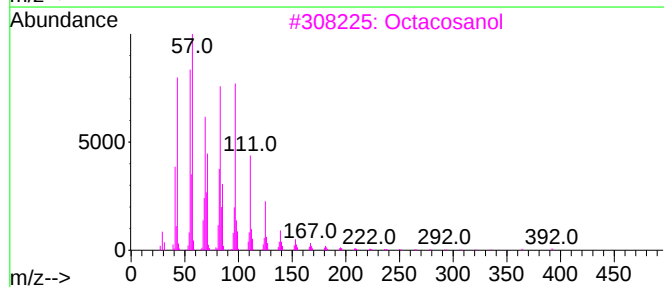
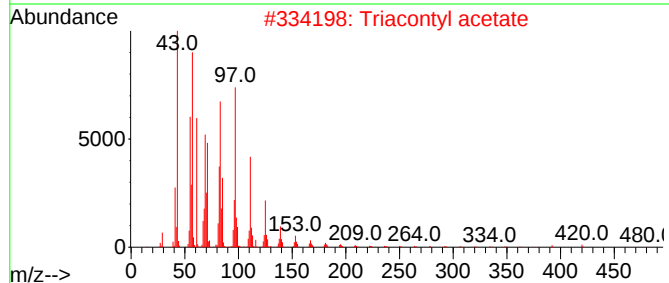
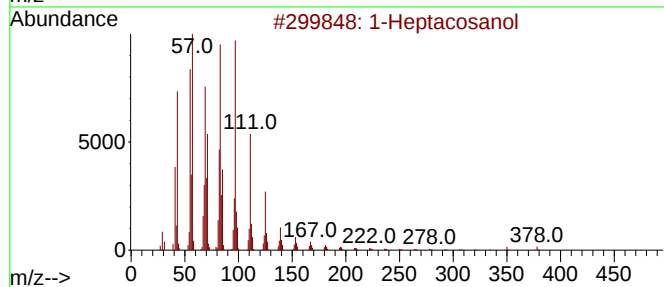
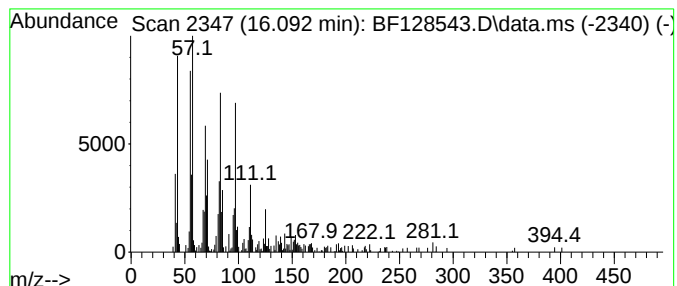
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.092	7.16 ng	352492	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Triacontyl acetate	480	C32H64O2	041755-58-2	94
3	Octacosanol	410	C28H58O	000557-61-9	94
4	Fumaric acid, hexadecyl 2-methyl...	394	C24H42O4	1000330-55-5	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128543.D
Acq On : 28 May 2022 12:33
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P026-SS001-0006-01

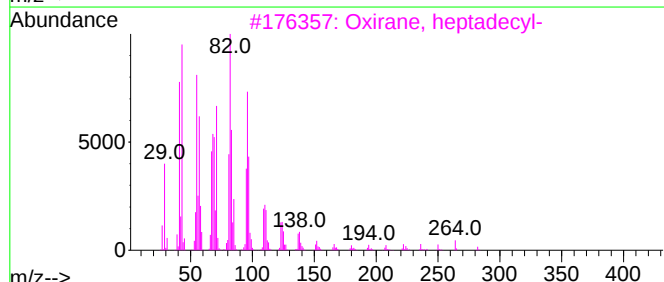
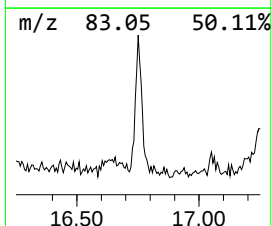
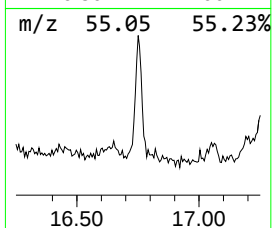
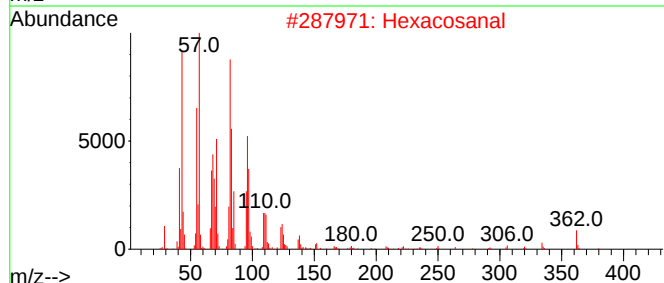
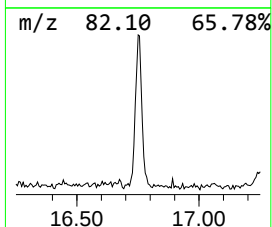
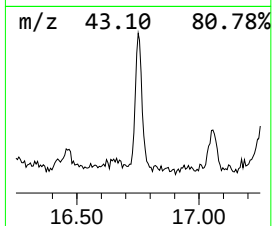
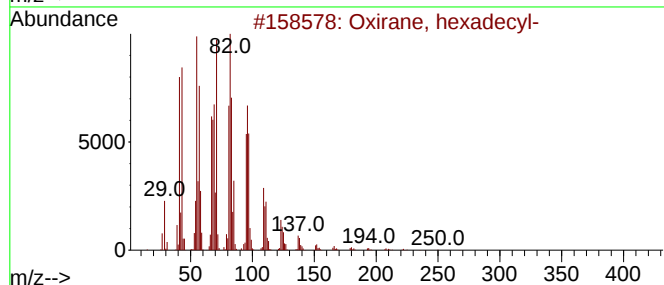
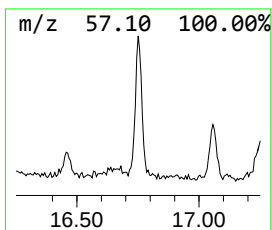
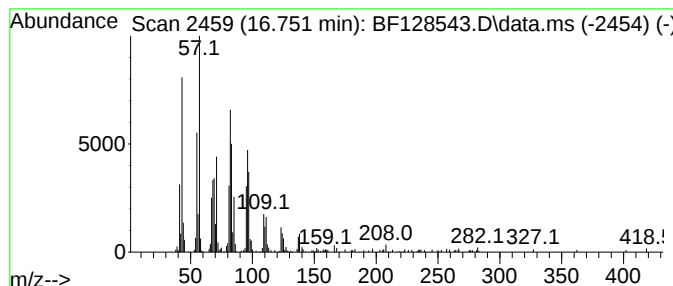
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Oxirane, hexadecyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.751	6.16 ng	303340	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
2		Hexacosanal	380	C26H52O	026627-85-0	87
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	72
4		Tetracosanal	352	C24H48O	057866-08-7	68
5		Octadecanal	268	C18H36O	000638-66-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128543.D
Acq On : 28 May 2022 12:33
Operator : CG\JU
Sample : N2928-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P026-SS001-0006-01

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
unknown6.287	6.287	3.9	ng	239575	1	6.834	1244420	20.0
unknown6.575	6.575	4.9	ng	305532	1	6.834	1244420	20.0
n-Hexadecanoic ...	11.892	5.0	ng	464473	4	11.363	1864930	20.0
1,1'-Biphenyl, ...	12.674	3.3	ng	308085	4	11.363	1864930	20.0
2,3,4,4',5,6-He...	13.539	2.9	ng	183465	5	13.998	1259650	20.0
1-Tetracosene	13.898	6.0	ng	381042	5	13.998	1259650	20.0
Triphenylphosph...	14.098	7.5	ng	473786	5	13.998	1259650	20.0
Nonadecanoic ac...	15.098	2.4	ng	116722	6	15.468	984153	20.0
Tetradecane, 1-...	15.133	3.6	ng	177987	6	15.468	984153	20.0
Octacosane	15.951	2.9	ng	140910	6	15.468	984153	20.0
1-Heptacosanol	16.092	7.2	ng	352492	6	15.468	984153	20.0
Oxirane, hexade...	16.751	6.2	ng	303340	6	15.468	984153	20.0