

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
 Data File : BF129977.D
 Acq On : 24 Aug 2022 17:57
 Operator : CG\JU
 Sample : N4244-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-103I

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-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.487	31	34	43	rBV	31893	50178	1.28%	0.265%
2	4.981	455	458	469	rBV	98656	130866	3.33%	0.692%
3	5.404	527	530	552	rBV	1280229	1556381	39.59%	8.233%
4	6.428	701	704	720	rBV	879393	955156	24.30%	5.053%
5	6.763	758	761	770	rBV	726284	646897	16.46%	3.422%
6	7.339	854	859	862	rBV	2292274	2162379	55.01%	11.438%
7	8.045	976	979	988	rBV	1004171	856976	21.80%	4.533%
8	9.122	1157	1162	1165	rBV	4733772	3931200	100.00%	20.795%
9	9.798	1274	1277	1281	rVB	1114052	914977	23.27%	4.840%
10	10.598	1409	1413	1416	rBV	2501720	2317906	58.96%	12.261%
11	11.292	1527	1531	1534	rBV	905654	819180	20.84%	4.333%
12	11.810	1616	1619	1622	rBV3	101684	116365	2.96%	0.616%
13	12.733	1772	1776	1780	rBV	59782	83353	2.12%	0.441%
14	12.874	1795	1800	1803	rBV	3175674	2663931	67.76%	14.091%
15	13.780	1946	1954	1967	rBV3	61800	210816	5.36%	1.115%
16	13.933	1977	1980	1990	rVB	589381	586211	14.91%	3.101%
17	14.021	1990	1995	2000	rBV	96173	114370	2.91%	0.605%
18	14.074	2000	2004	2006	rVB	49587	48827	1.24%	0.258%
19	14.374	2052	2055	2059	rBV	75227	67672	1.72%	0.358%
20	14.674	2102	2106	2111	rVB	66784	69813	1.78%	0.369%
21	14.998	2157	2161	2166	rVB	46212	57799	1.47%	0.306%
22	15.386	2223	2227	2234	rVB	457546	543308	13.82%	2.874%

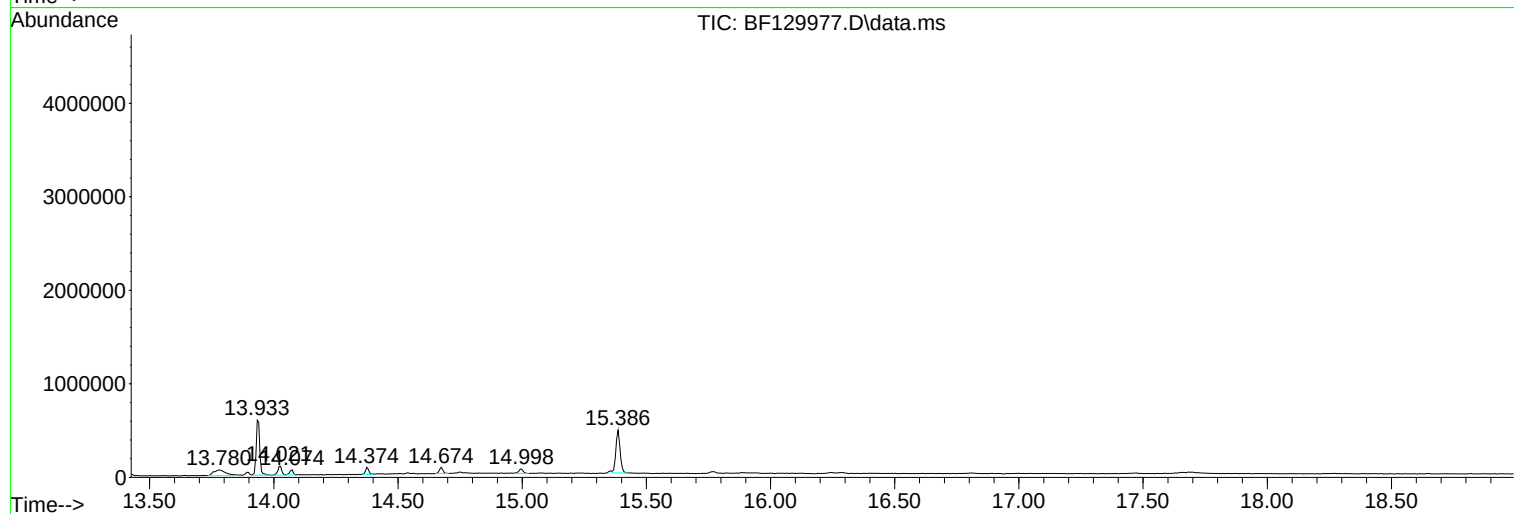
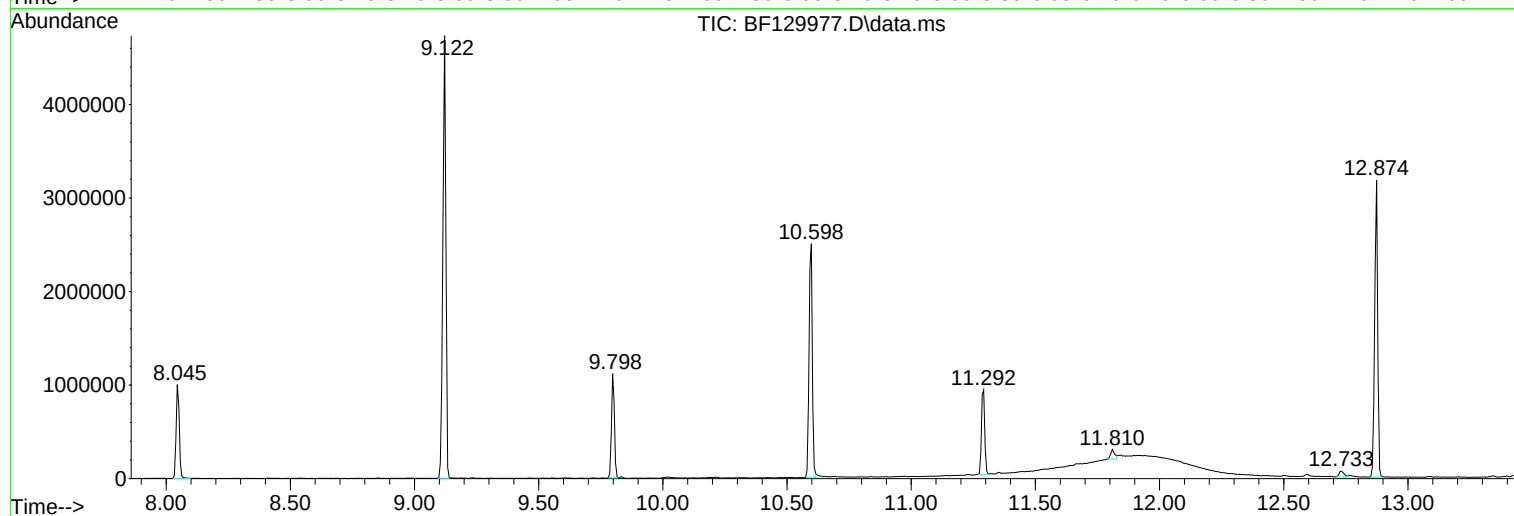
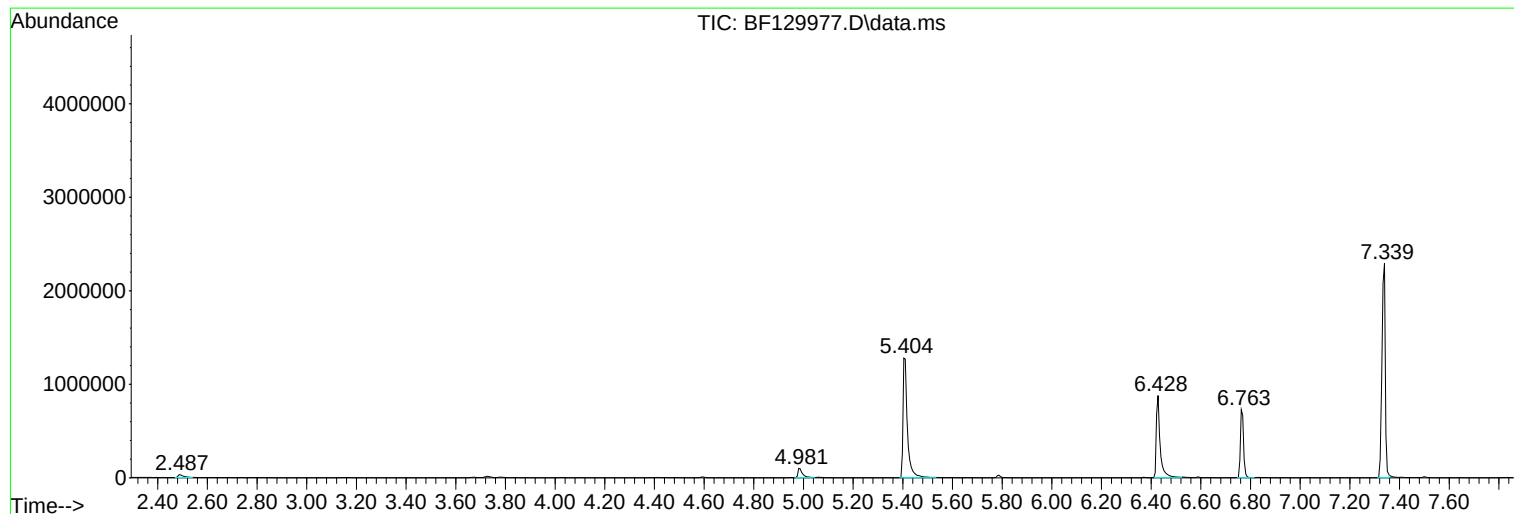
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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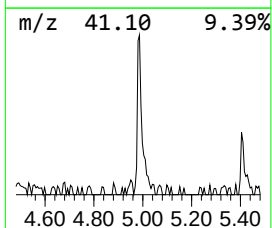
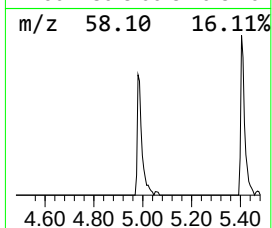
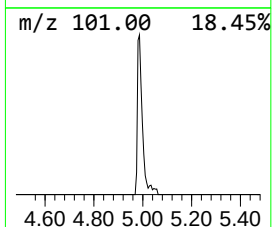
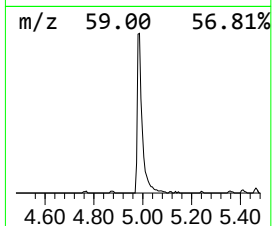
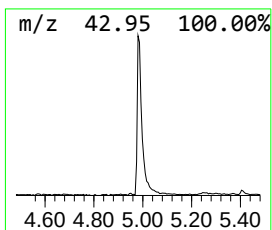
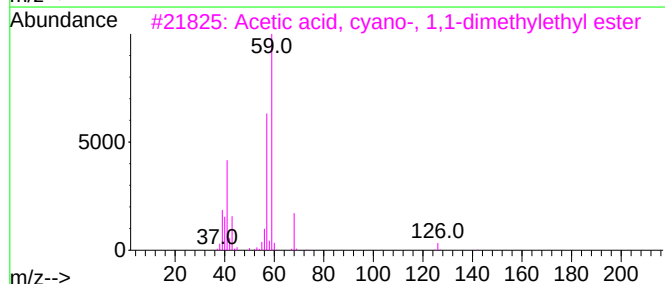
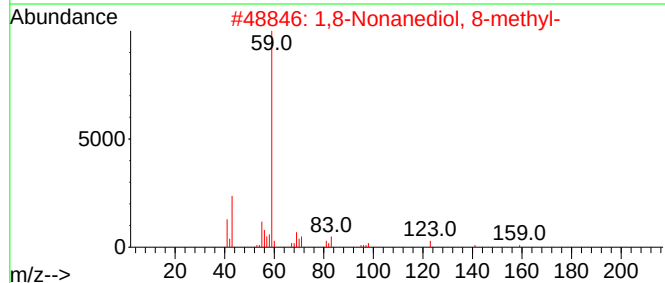
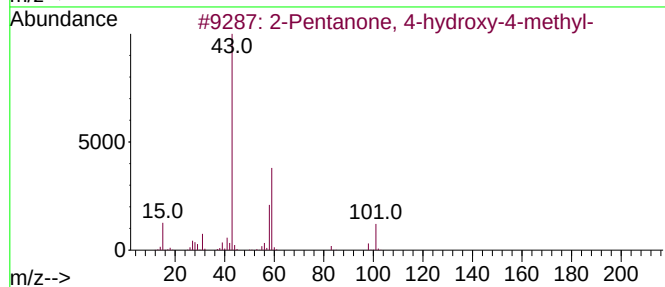
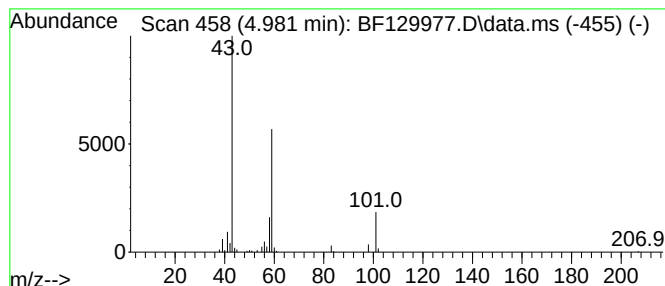
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	4.05 ng	130866	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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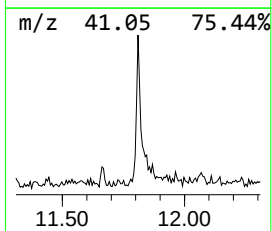
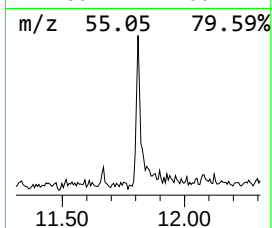
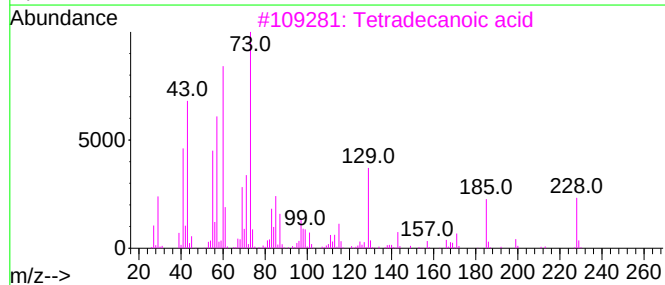
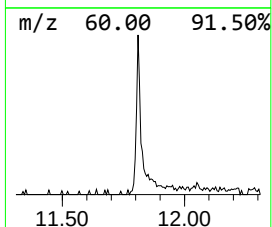
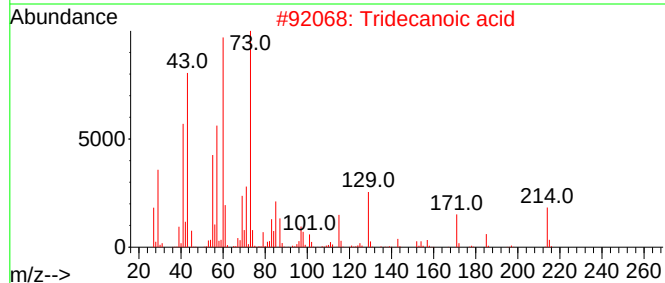
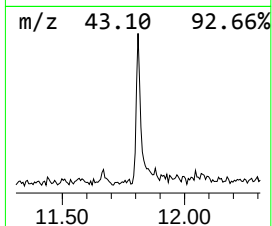
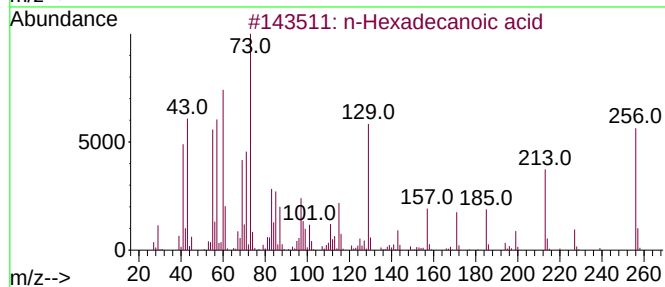
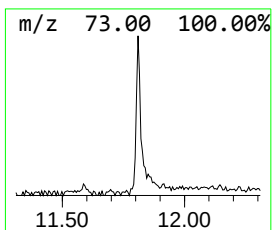
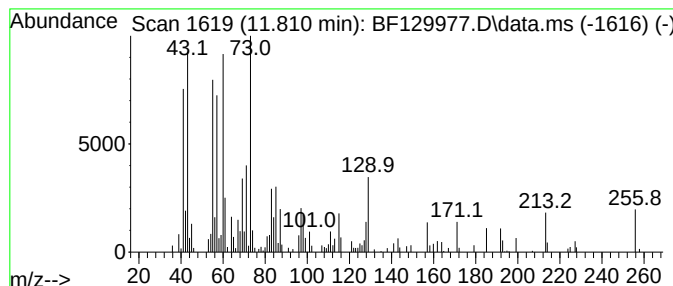
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.810	2.84 ng	116365	Phenanthrene-d10		11.292	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	83
5	Dodecanoic acid		200	C12H24O2	000143-07-7	80



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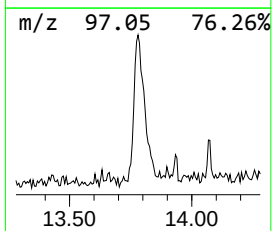
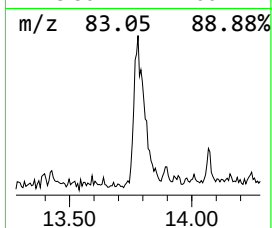
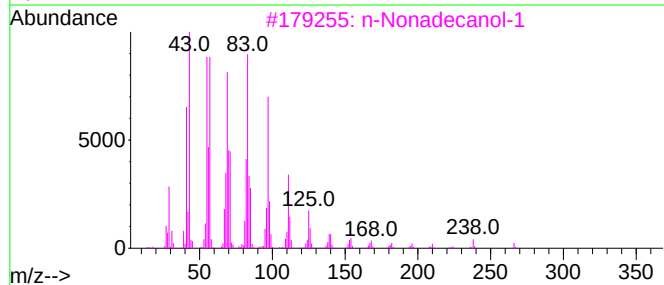
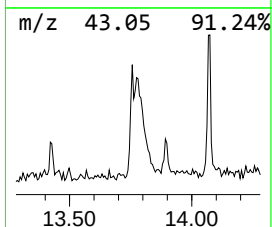
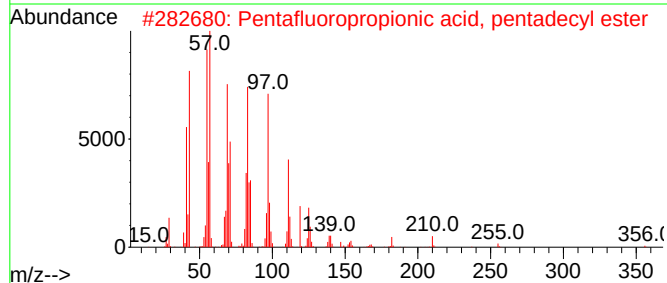
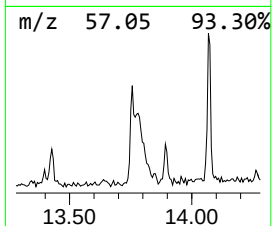
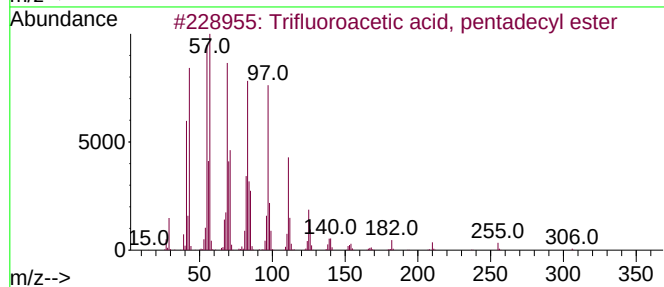
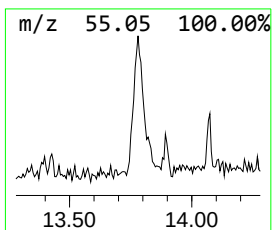
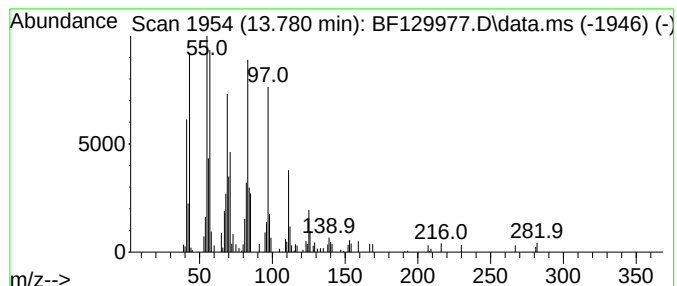
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Peak Number 3 Trifluoroacetic acid, penta... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	7.19 ng	210816	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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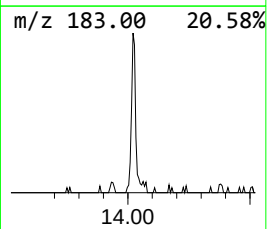
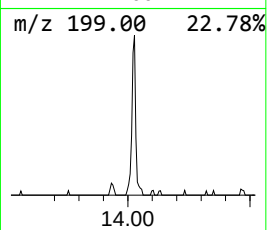
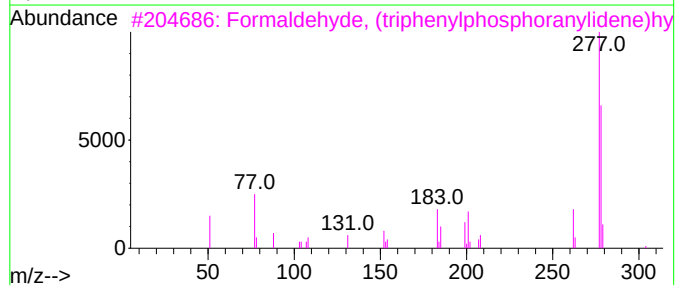
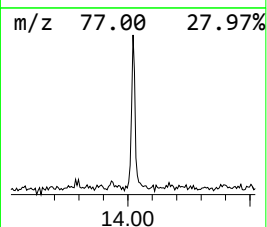
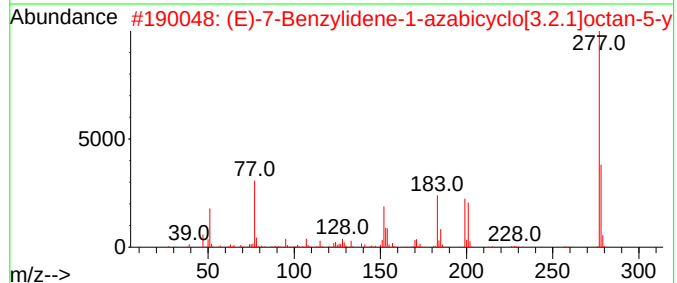
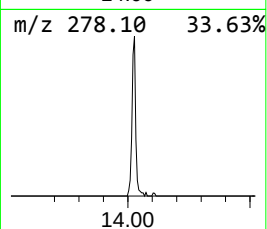
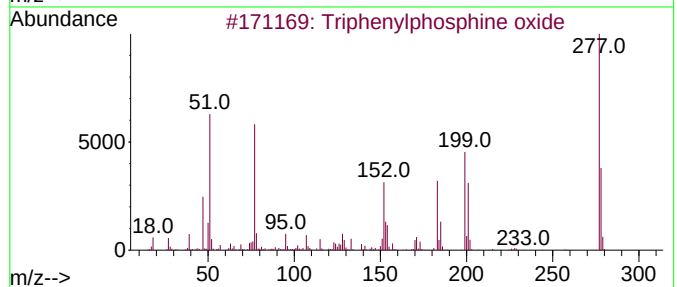
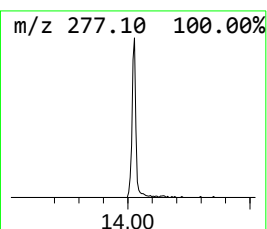
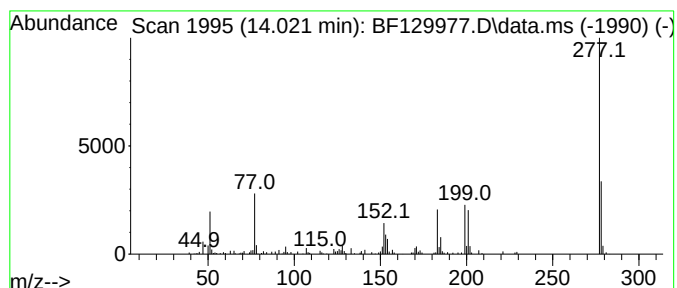
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.021	3.90 ng	114370	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	27



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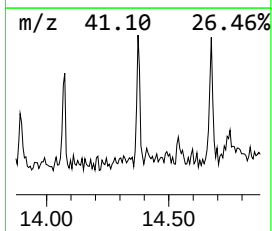
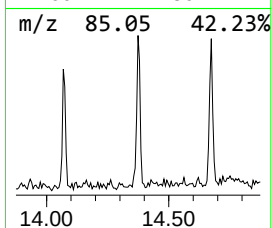
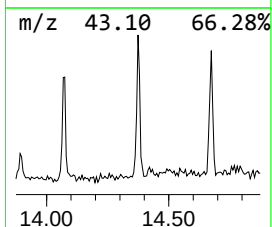
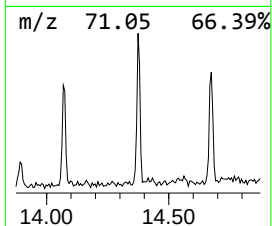
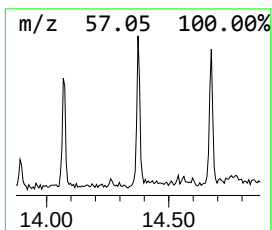
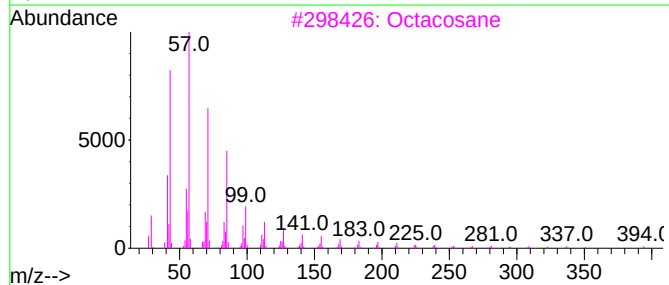
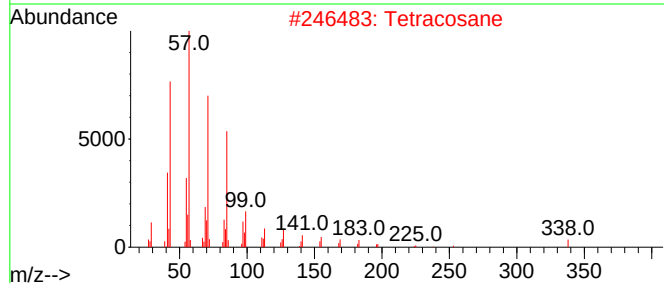
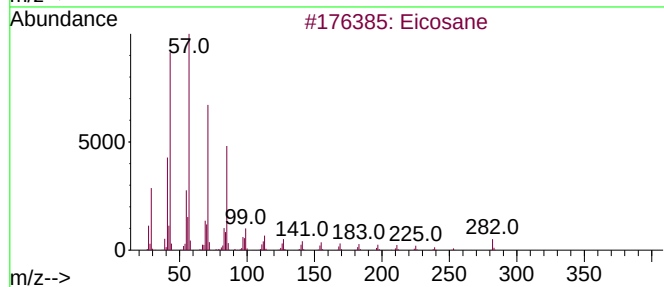
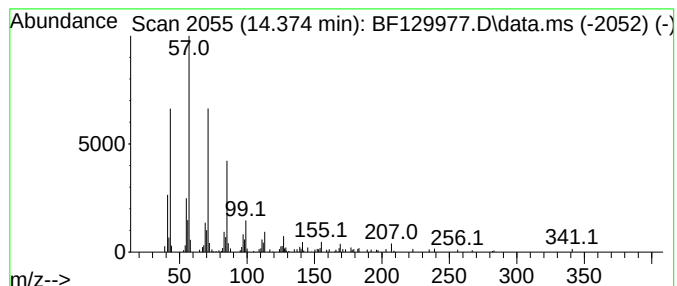
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.374	2.31 ng	67672	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Tetracosane	338	C24H50	000646-31-1	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Pentacosane	352	C25H52	000629-99-2	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



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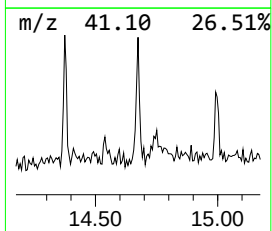
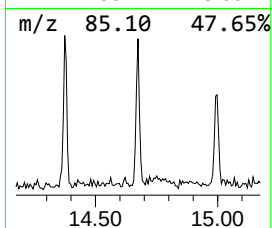
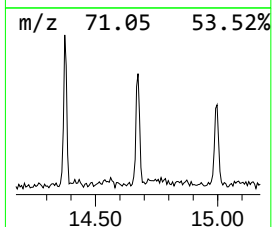
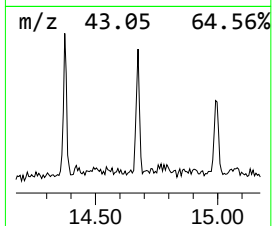
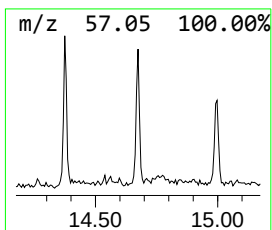
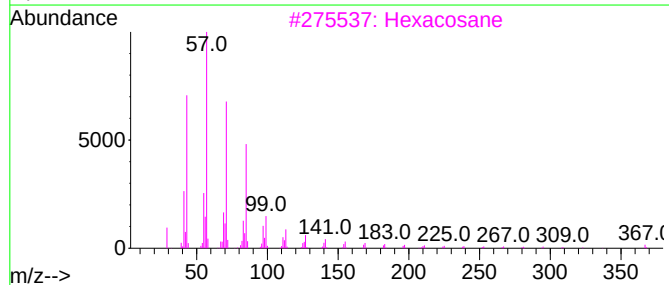
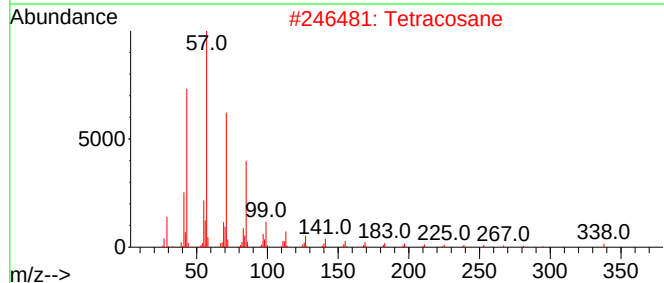
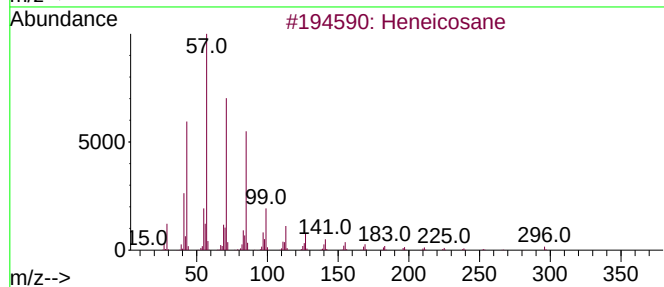
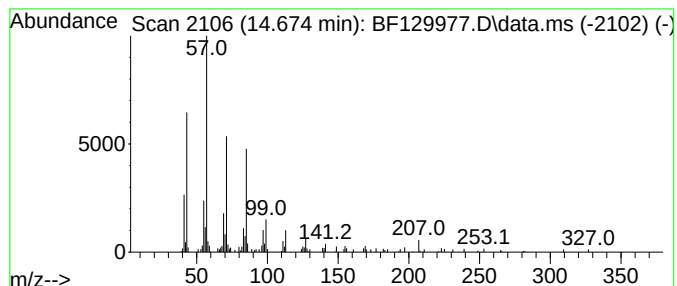
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.674	2.57 ng	69813	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129977.D
Acq On : 24 Aug 2022 17:57
Operator : CG\JU
Sample : N4244-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103I

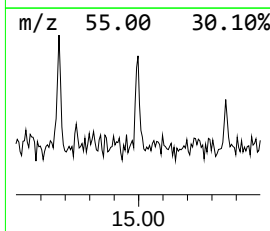
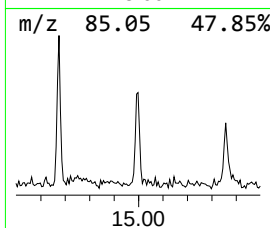
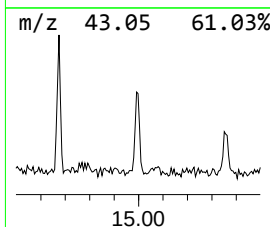
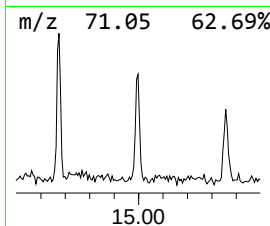
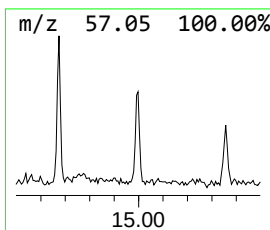
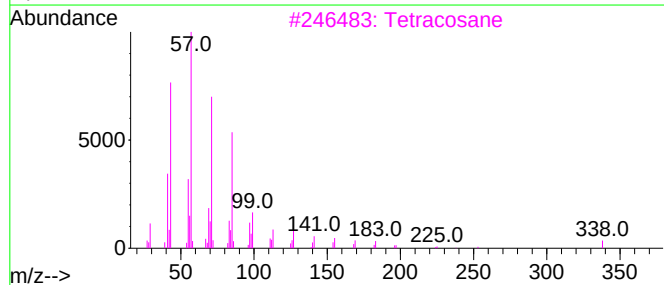
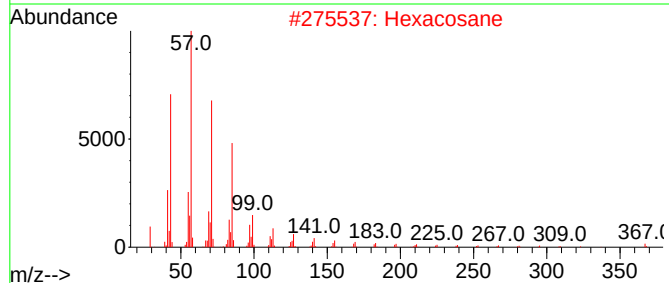
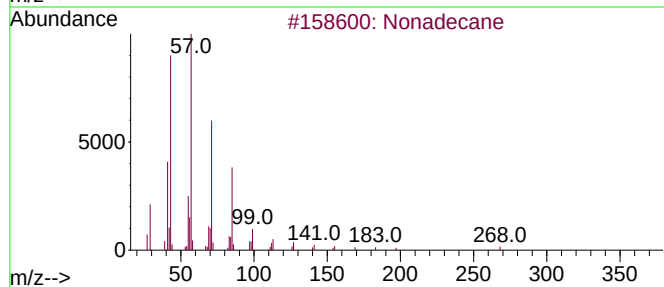
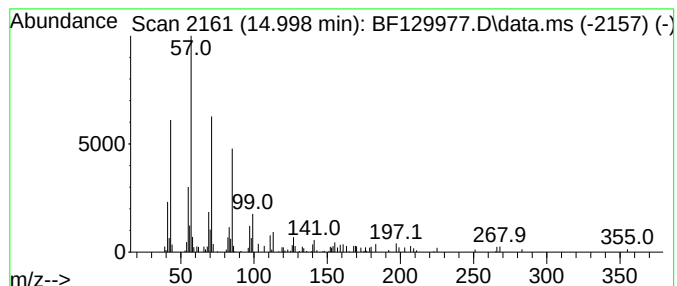
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	2.13 ng	57799	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Hexacosane	366	C26H54	000630-01-3	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129977.D
Acq On : 24 Aug 2022 17:57
Operator : CG\JU
Sample : N4244-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-103I

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	4.0	ng	130866	1	6.763	646897	20.0
n-Hexadecanoic ...	11.810	2.8	ng	116365	4	11.292	819180	20.0
Trifluoroacetic...	13.780	7.2	ng	210816	5	13.933	586211	20.0
Triphenylphosph...	14.021	3.9	ng	114370	5	13.933	586211	20.0
Eicosane	14.374	2.3	ng	67672	5	13.933	586211	20.0
Heneicosane	14.674	2.6	ng	69813	6	15.386	543308	20.0
Nonadecane	14.998	2.1	ng	57799	6	15.386	543308	20.0