

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
 Data File : BF129976.D
 Acq On : 24 Aug 2022 17:20
 Operator : CG\JU
 Sample : N4229-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-106S

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: BF129976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	455	458	469	rBV	74498	92658	2.92%	0.588%
2	5.404	527	530	551	rBV	1003148	1225371	38.58%	7.770%
3	6.428	701	704	718	rBV	651419	719125	22.64%	4.560%
4	6.763	758	761	769	rBV	667233	575184	18.11%	3.647%
5	7.334	854	858	868	rBV	2000593	1856115	58.44%	11.769%
6	8.045	976	979	989	rBV	920201	741532	23.35%	4.702%
7	9.122	1157	1162	1165	rBV	3797967	3176081	100.00%	20.139%
8	9.798	1273	1277	1281	rBV	955950	766028	24.12%	4.857%
9	10.010	1309	1313	1322	rBV7	18958	39757	1.25%	0.252%
10	10.592	1409	1412	1423	rBV	1939290	1747701	55.03%	11.082%
11	11.286	1527	1530	1534	rBV	724137	647826	20.40%	4.108%
12	11.810	1614	1619	1622	rBV	148638	177615	5.59%	1.126%
13	12.592	1748	1752	1762	rBV	75558	100654	3.17%	0.638%
14	12.733	1772	1776	1783	rVB	50786	73216	2.31%	0.464%
15	12.874	1795	1800	1803	rBV	2720053	2478786	78.05%	15.718%
16	13.892	1969	1973	1977	rBV	70099	68897	2.17%	0.437%
17	13.933	1977	1980	1989	rVB	544069	502022	15.81%	3.183%
18	14.027	1991	1996	2000	rVV	76085	81737	2.57%	0.518%
19	14.068	2000	2003	2009	rVV	39163	42470	1.34%	0.269%
20	14.374	2052	2055	2059	rVB	49023	44437	1.40%	0.282%
21	14.486	2071	2074	2077	rBV	45417	42827	1.35%	0.272%
22	14.674	2102	2106	2111	rVB2	44712	53942	1.70%	0.342%
23	15.386	2223	2227	2234	rVB	426424	516806	16.27%	3.277%

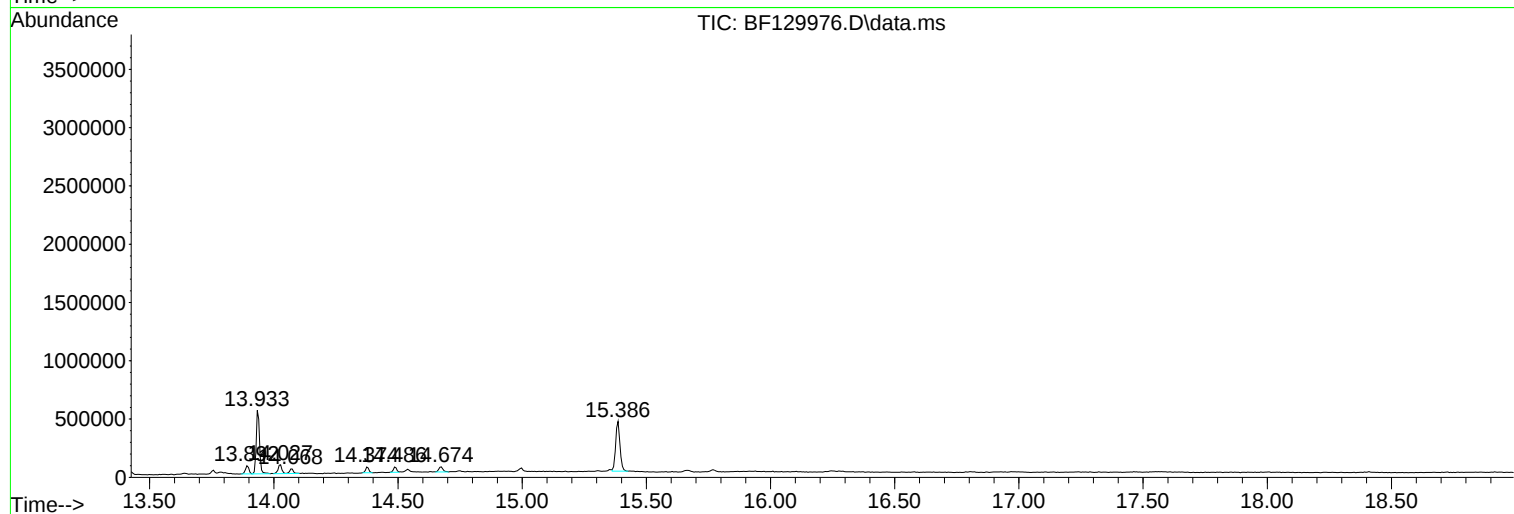
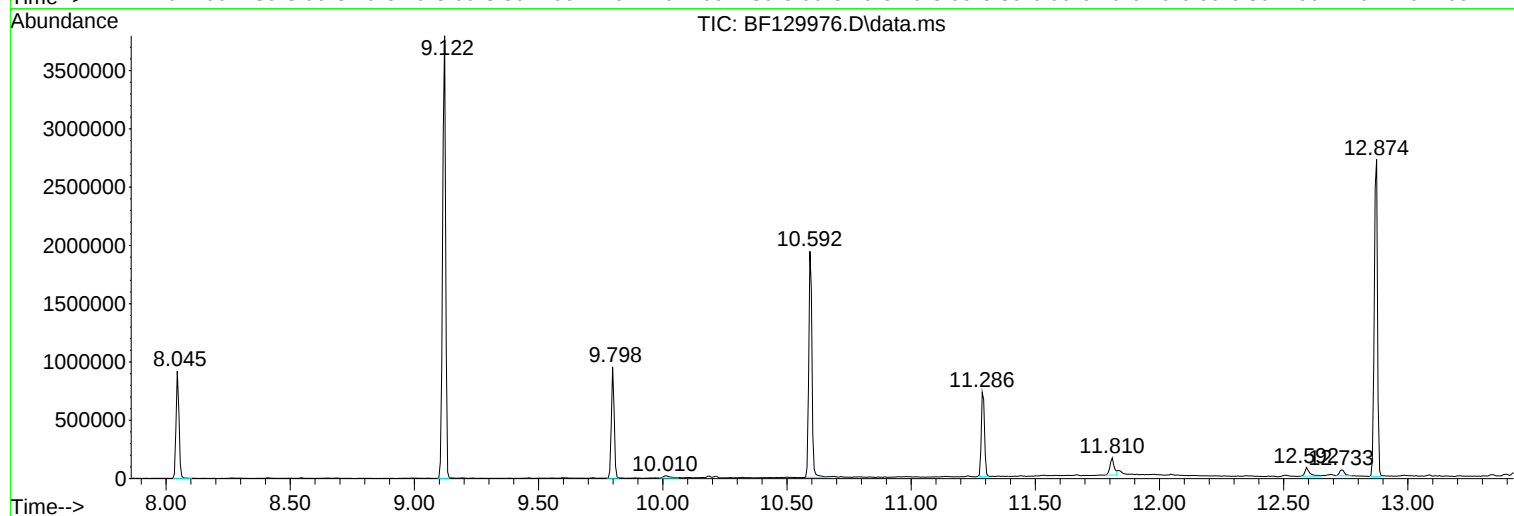
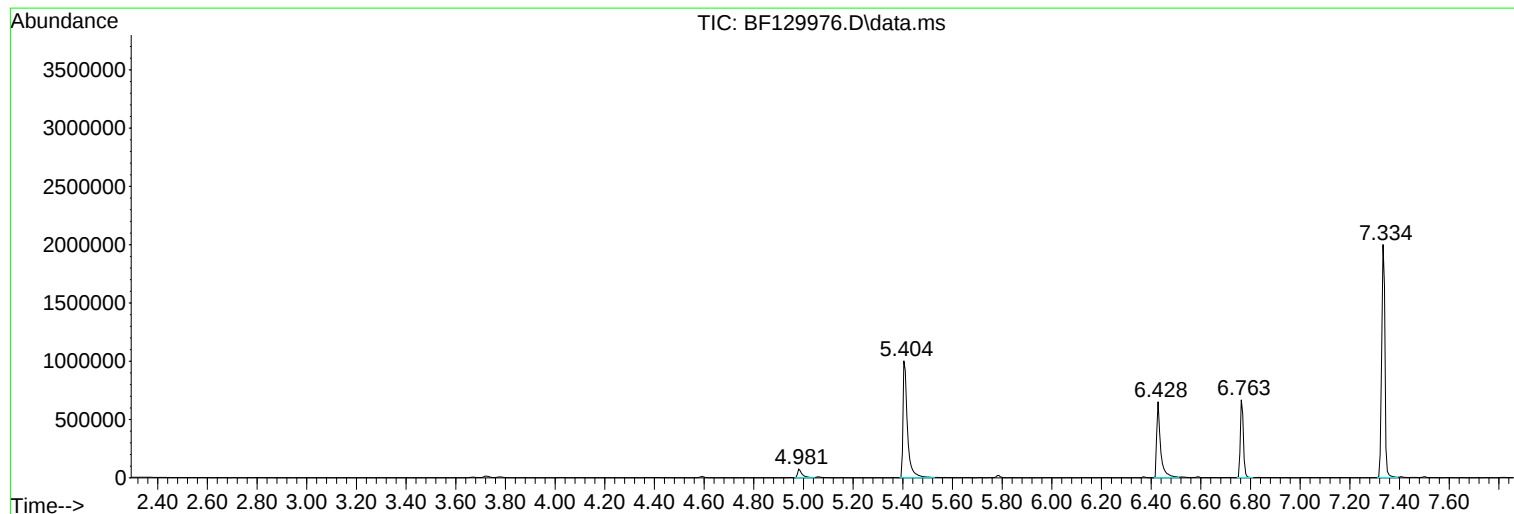
Sum of corrected areas: 15770787

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

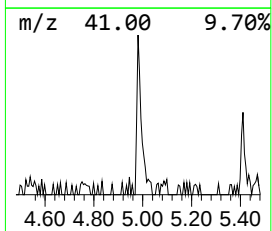
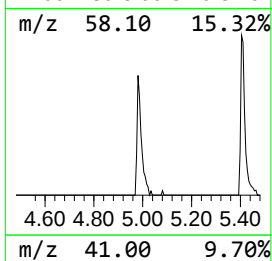
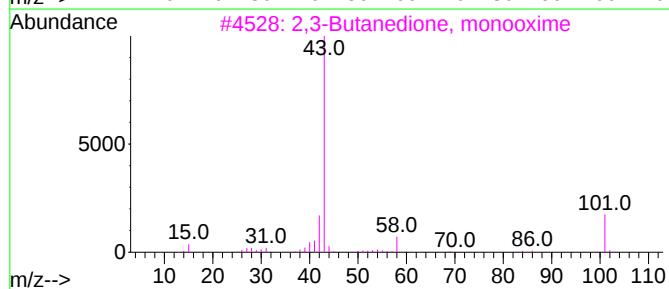
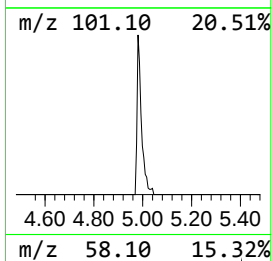
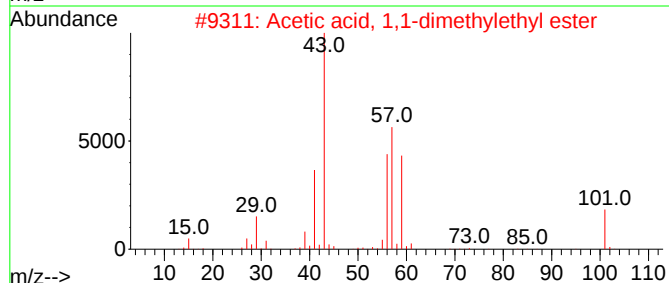
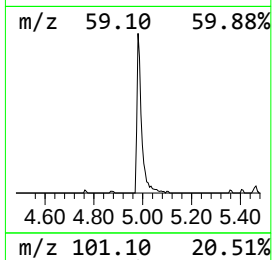
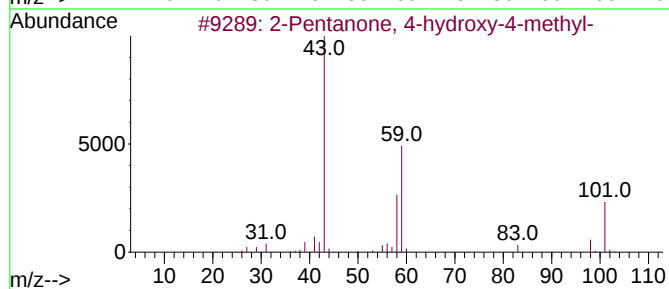
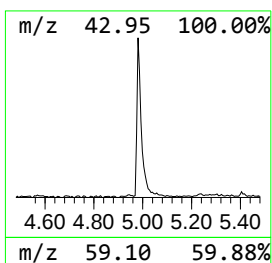
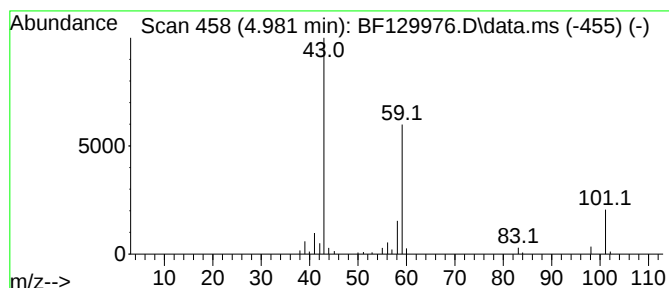
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	3.22 ng	92658	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	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

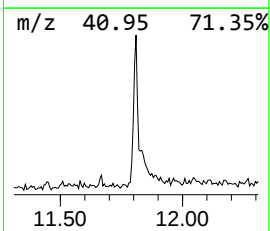
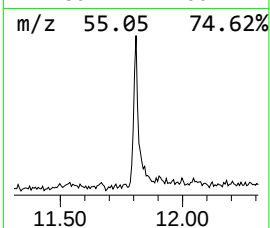
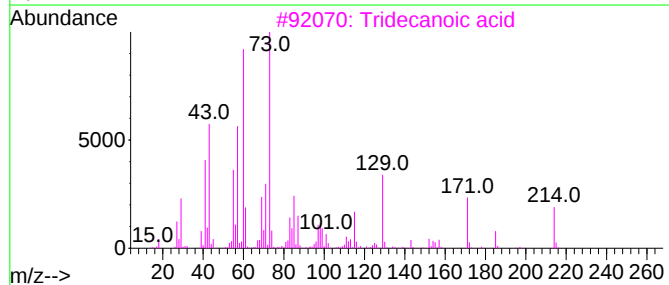
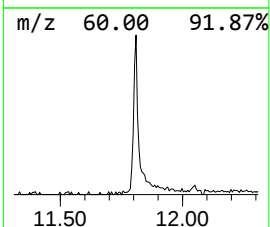
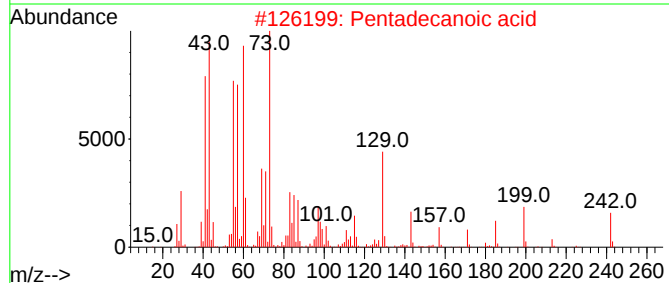
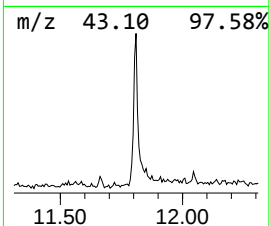
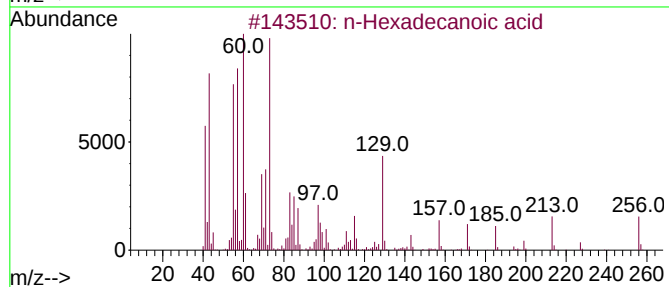
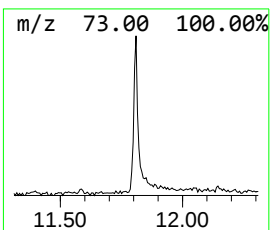
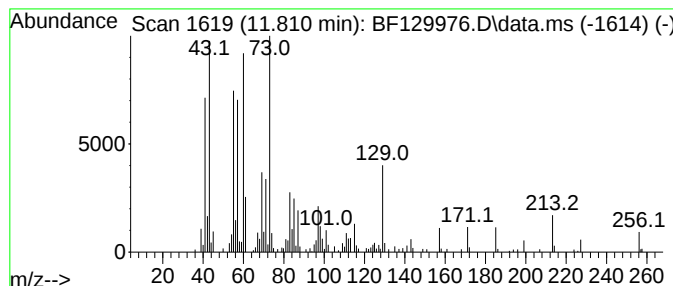
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	5.48 ng	177615	Phenanthrene-d10	11.286

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

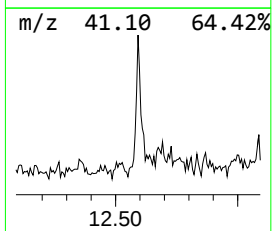
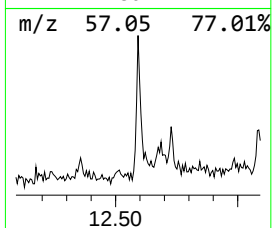
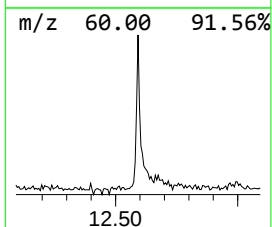
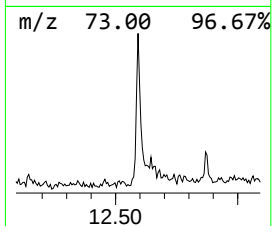
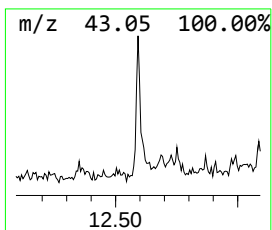
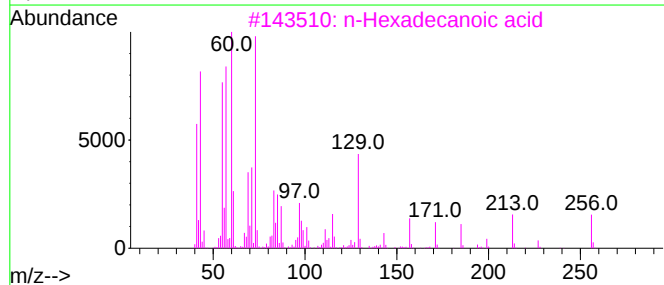
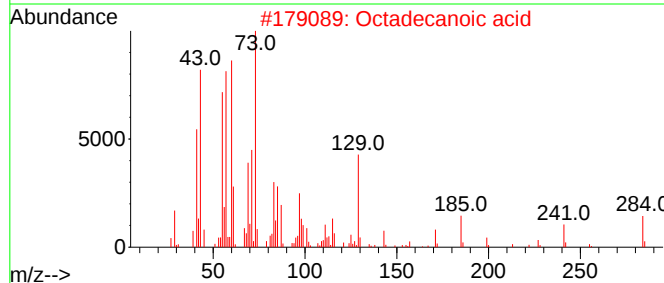
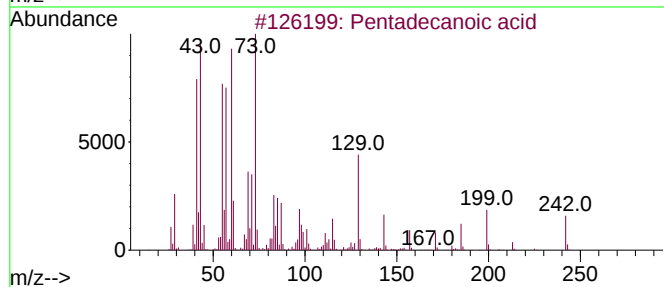
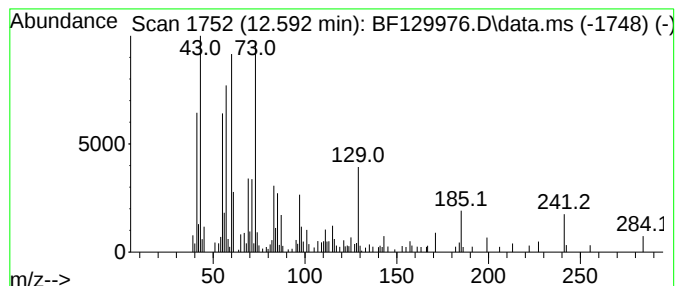
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	3.11 ng	100654	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

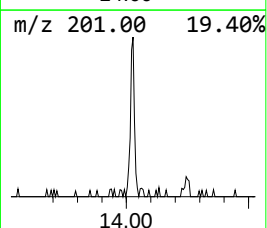
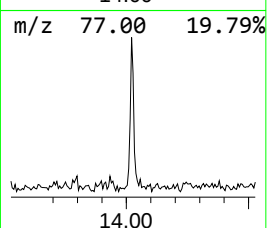
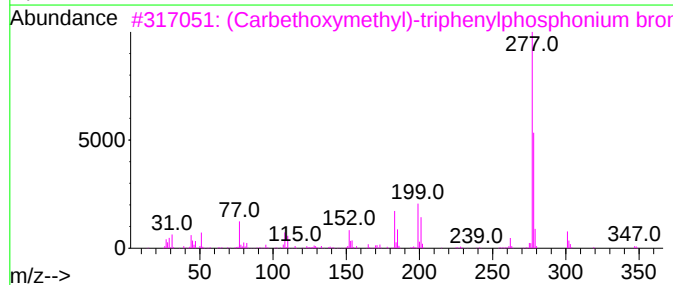
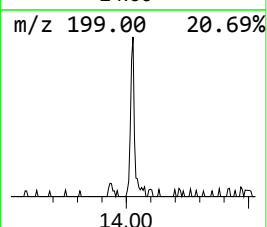
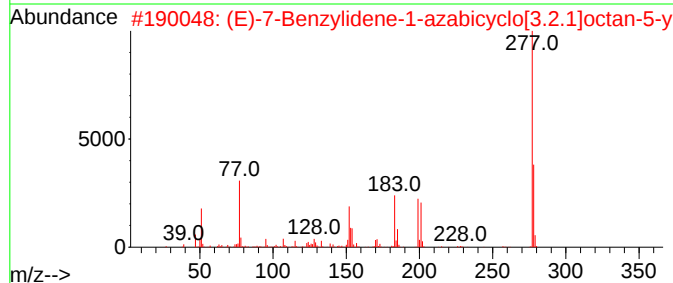
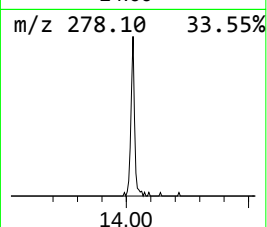
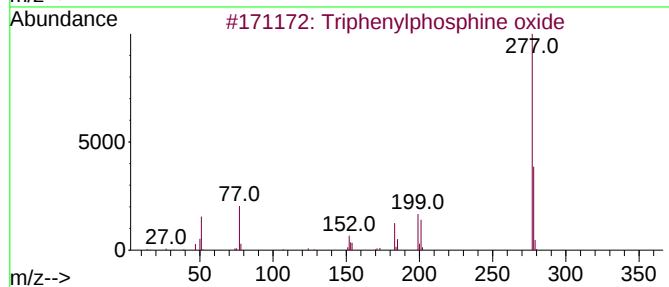
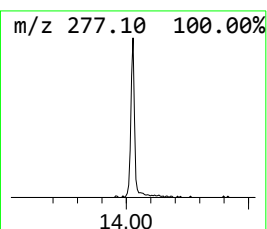
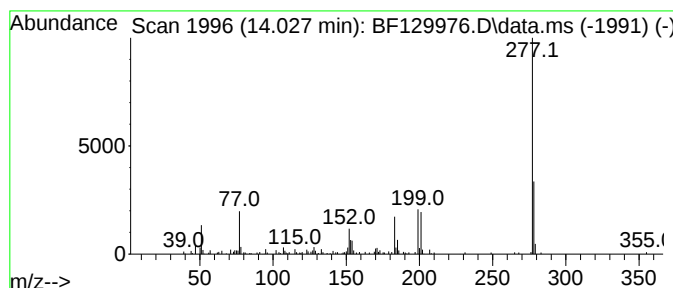
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	3.26 ng	81737	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

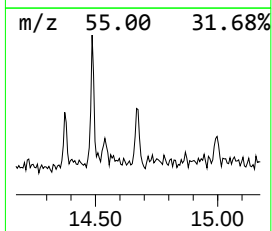
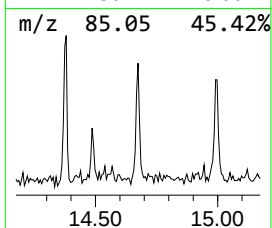
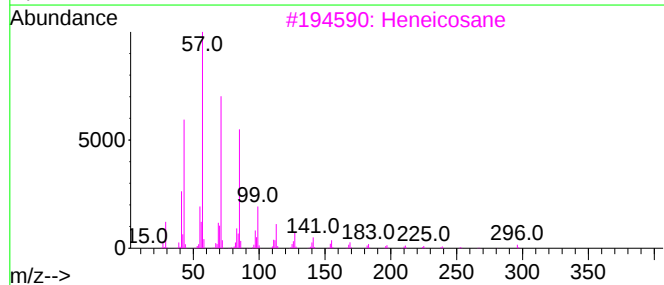
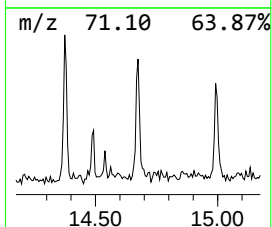
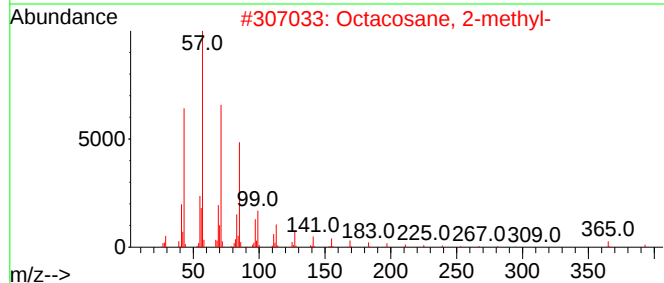
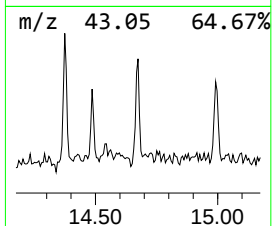
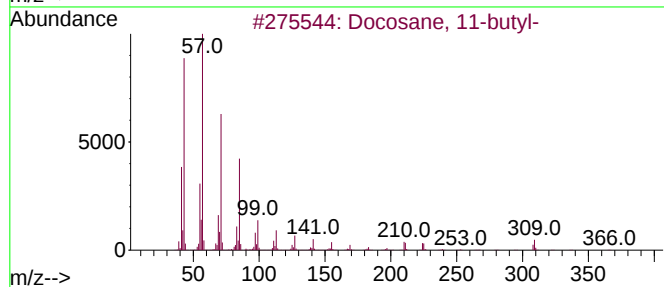
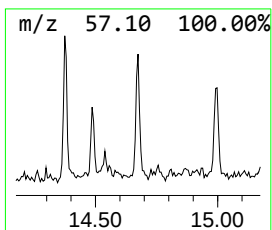
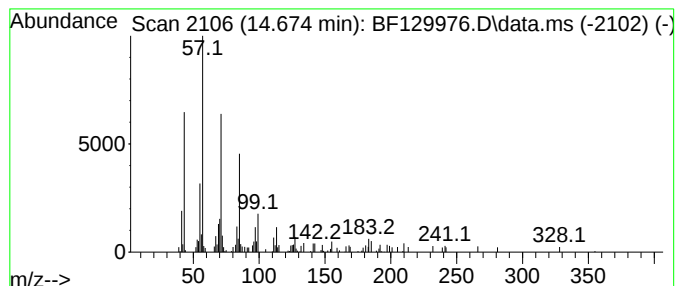
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Docosane, 11-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.674	2.09 ng	53942	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Hentriacontane	437	C31H64	000630-04-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082422\
Data File : BF129976.D
Acq On : 24 Aug 2022 17:20
Operator : CG\JU
Sample : N4229-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-106S

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	3.2	ng	92658	1	6.763	575184	20.0
n-Hexadecanoic ...	11.810	5.5	ng	177615	4	11.286	647826	20.0
Pentadecanoic acid	12.592	3.1	ng	100654	4	11.286	647826	20.0
Triphenylphosph...	14.027	3.3	ng	81737	5	13.933	502022	20.0
Docosane, 11-bu...	14.674	2.1	ng	53942	6	15.386	516806	20.0