

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
 Data File : BF127600.D
 Acq On : 31 Mar 2022 13:11
 Operator : CG\JU
 Sample : N2171-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PSE-COMP-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-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	471	474	487	rBV	55060	77702	3.08%	0.431%
2	5.469	538	541	562	rBV	2154718	2279016	90.40%	12.636%
3	6.475	709	712	730	rBV	2062952	2363991	93.77%	13.107%
4	6.834	770	773	781	rBV	626409	512676	20.33%	2.842%
5	7.404	865	870	880	rBV	1507552	1571544	62.33%	8.713%
6	8.028	972	976	982	rBV2	24555	41831	1.66%	0.232%
7	8.116	987	991	999	rVV	703947	650251	25.79%	3.605%
8	9.186	1169	1173	1177	rBV	2568195	2521158	100.00%	13.978%
9	9.251	1182	1184	1190	rVB	30166	31186	1.24%	0.173%
10	9.869	1285	1289	1298	rBV	879051	737344	29.25%	4.088%
11	10.663	1421	1424	1438	rBV	1482207	1572198	62.36%	8.717%
12	11.363	1540	1543	1551	rBV	874576	748656	29.69%	4.151%
13	11.733	1603	1606	1610	rVB2	31607	30327	1.20%	0.168%
14	11.880	1627	1631	1635	rBV	44795	55873	2.22%	0.310%
15	12.122	1669	1672	1675	rVB	86513	63965	2.54%	0.355%
16	12.951	1808	1813	1816	rBV	2558033	2480503	98.39%	13.753%
17	13.157	1843	1848	1851	rBV	32210	29088	1.15%	0.161%
18	13.498	1903	1906	1909	rBV	79238	62981	2.50%	0.349%
19	13.827	1959	1962	1965	rBV	135268	163079	6.47%	0.904%
20	13.968	1983	1986	1990	rVB	31561	32333	1.28%	0.179%
21	14.016	1990	1994	2004	rBV	710502	690424	27.39%	3.828%
22	14.145	2012	2016	2019	rVB	150245	121197	4.81%	0.672%
23	14.451	2064	2068	2072	rBV	139754	119411	4.74%	0.662%
24	14.751	2116	2119	2123	rVB	104766	99403	3.94%	0.551%
25	14.827	2129	2132	2135	rBV	65995	63087	2.50%	0.350%
26	15.086	2172	2176	2181	rBV	73389	82990	3.29%	0.460%
27	15.462	2236	2240	2242	rBV3	36879	44621	1.77%	0.247%
28	15.498	2242	2246	2260	rVB	469547	655506	26.00%	3.634%
29	15.892	2309	2313	2318	rVB3	24471	34034	1.35%	0.189%
30	17.074	2507	2514	2523	rVB8	50231	100156	3.97%	0.555%

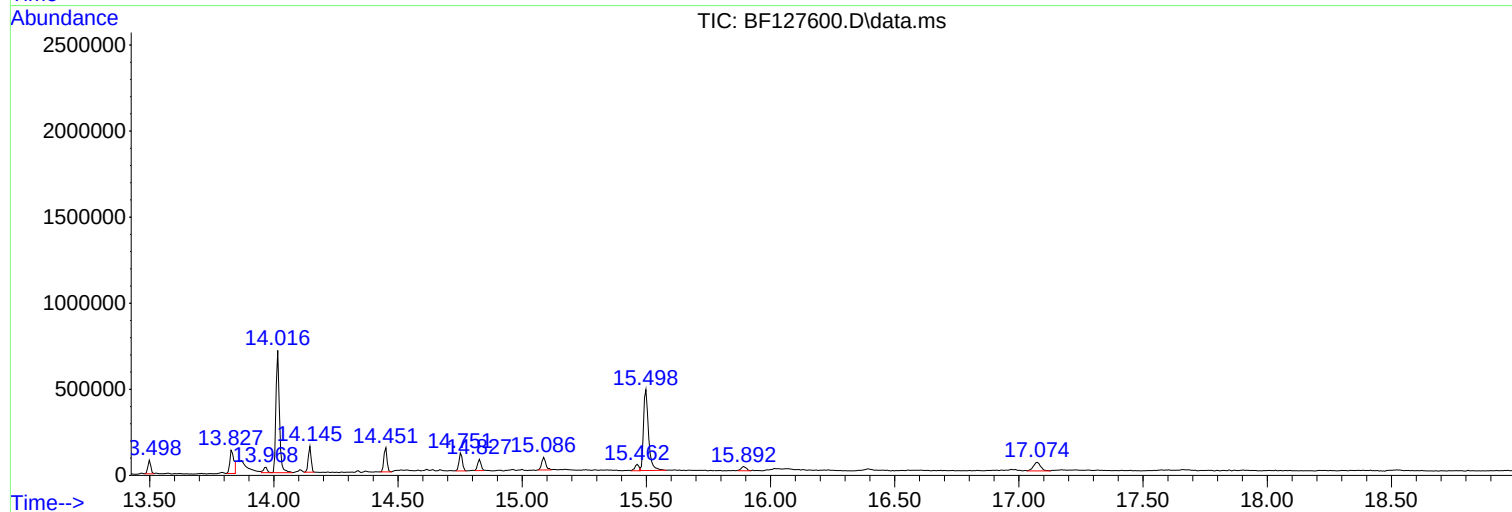
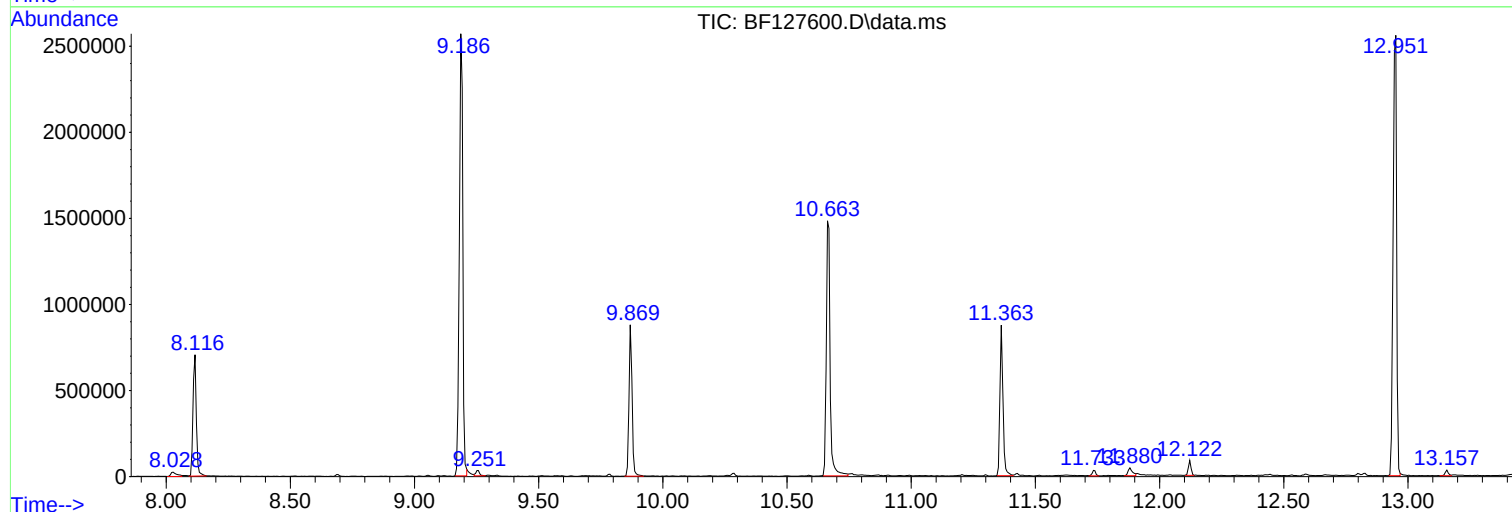
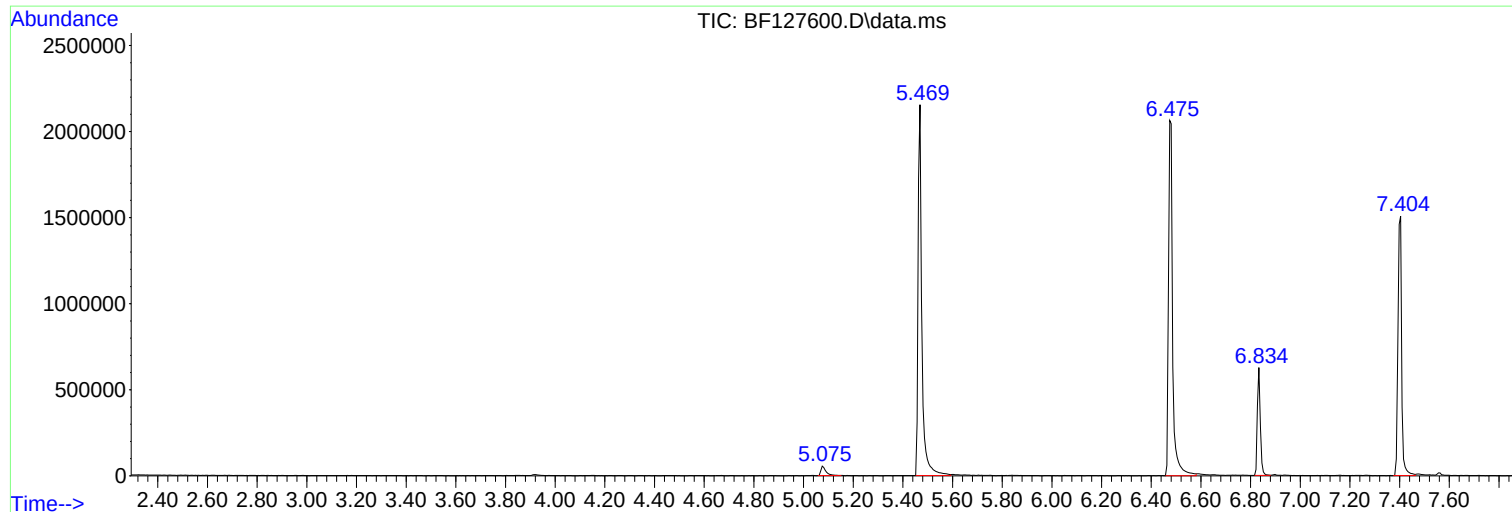
Sum of corrected areas: 18036531

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

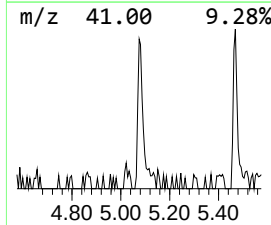
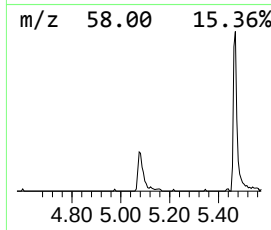
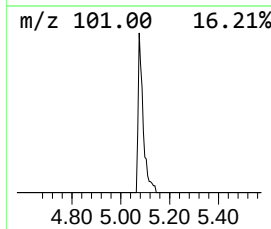
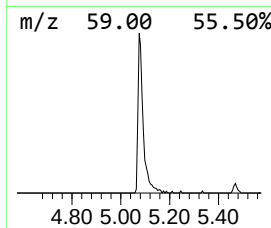
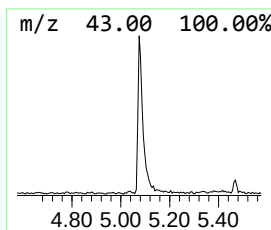
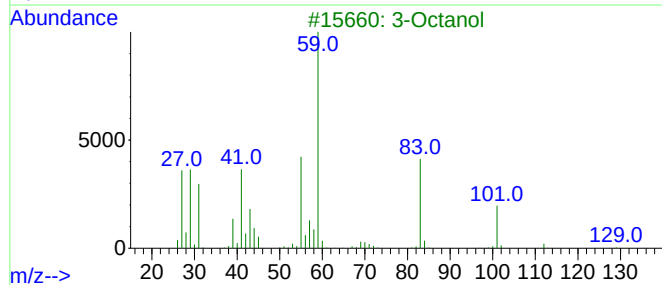
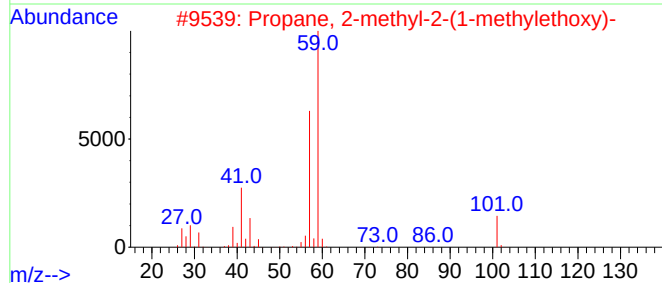
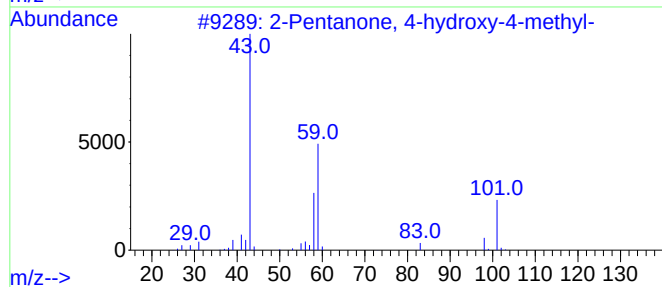
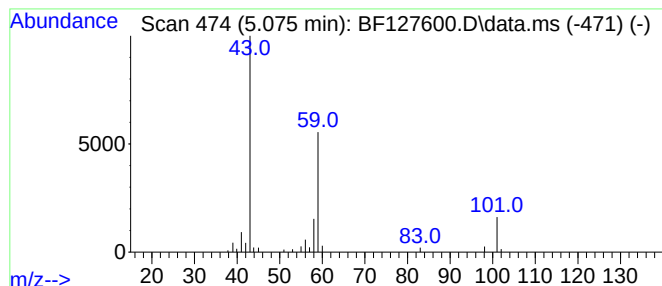
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.03 ng	77702	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

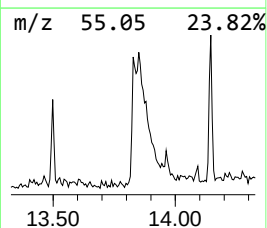
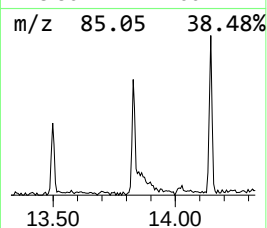
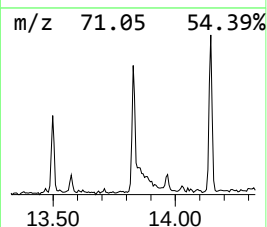
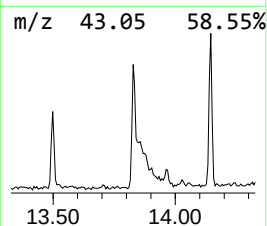
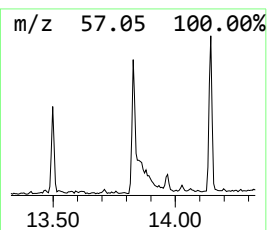
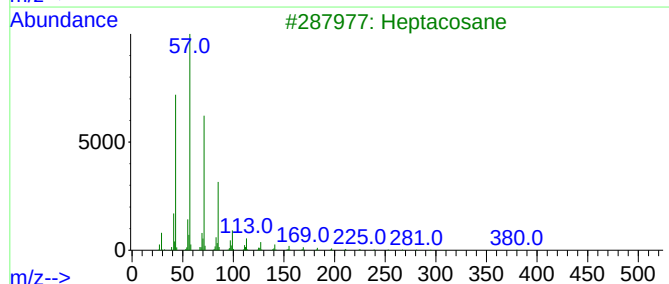
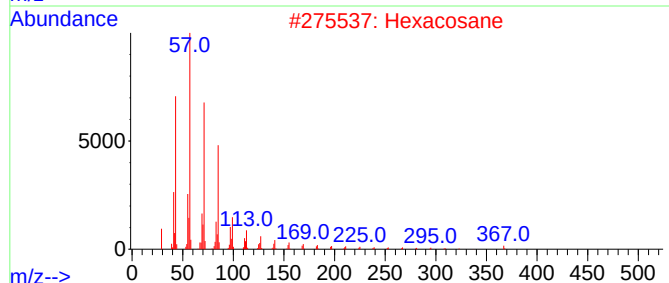
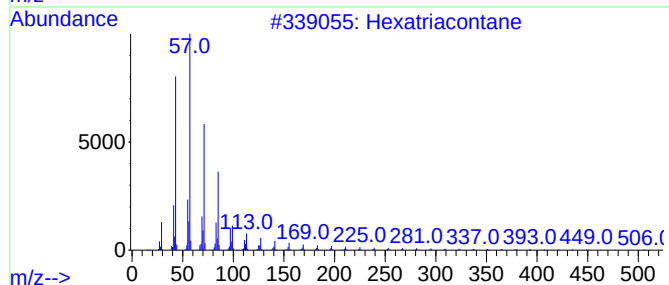
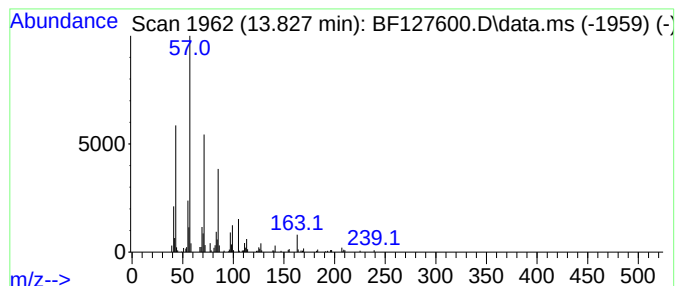
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexatriacontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.72 ng	163079	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	91
2			Hexacosane	366	C26H54	000630-01-3	87
3			Heptacosane	380	C27H56	000593-49-7	87
4			Nonadecane	268	C19H40	000629-92-5	81
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

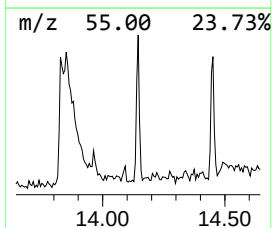
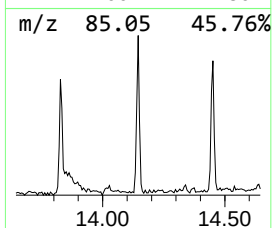
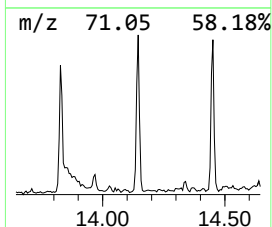
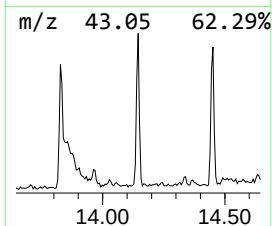
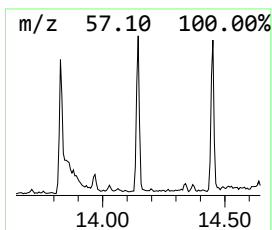
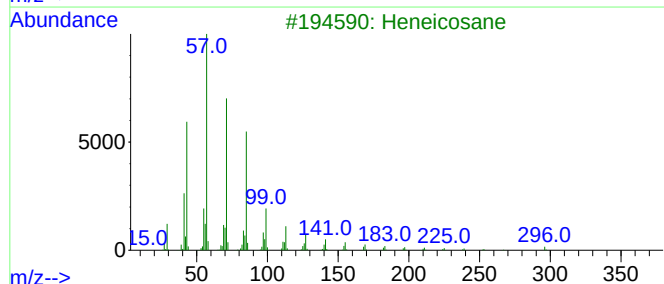
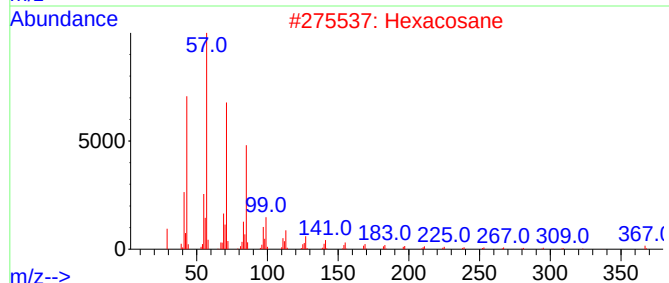
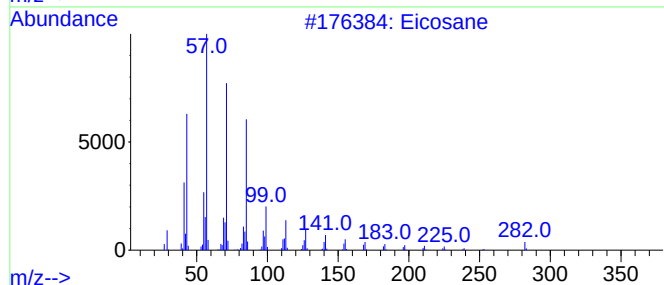
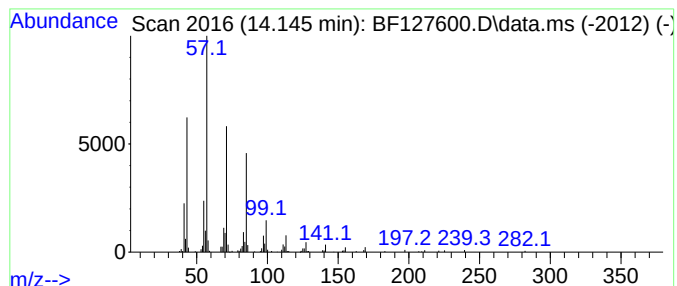
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	3.51 ng	121197	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Nonadecane	268	C19H40	000629-92-5	90
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

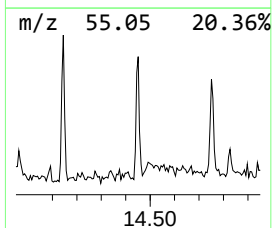
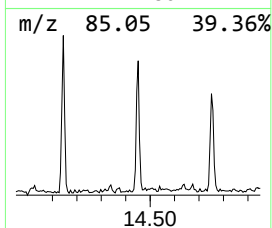
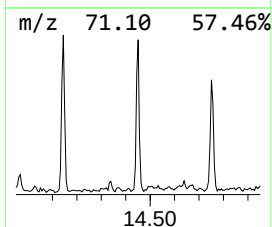
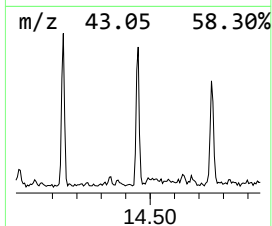
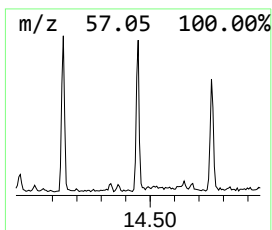
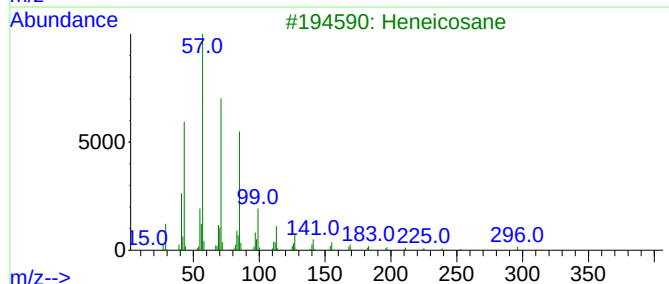
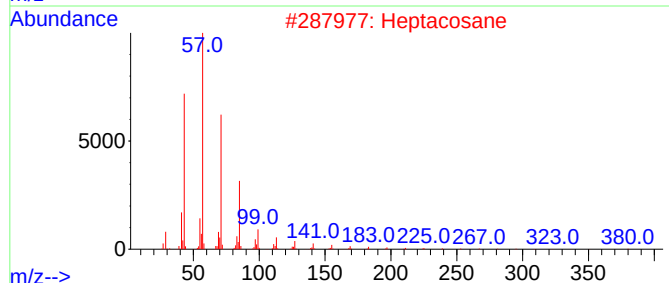
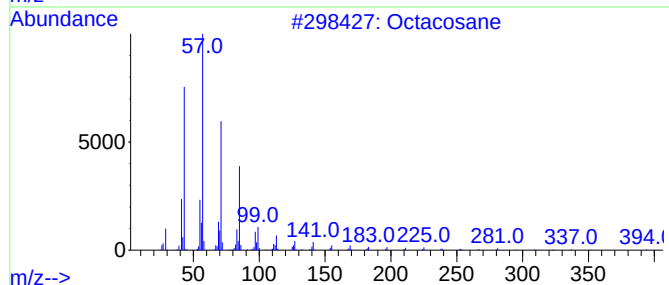
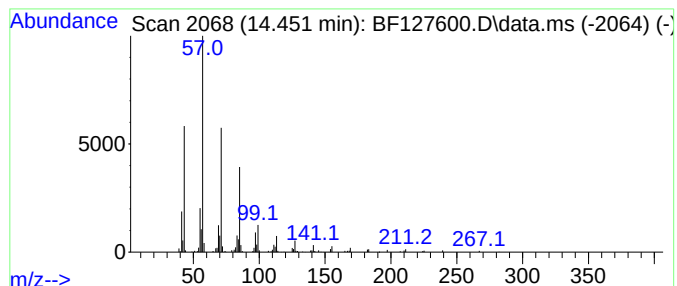
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	3.46 ng	119411	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Pentacosane	352	C25H52	000629-99-2	90
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

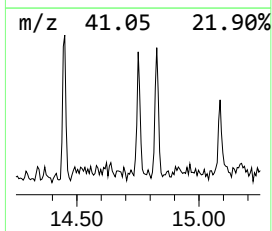
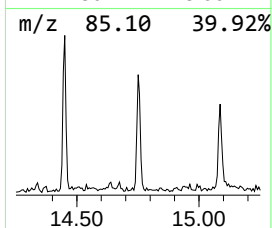
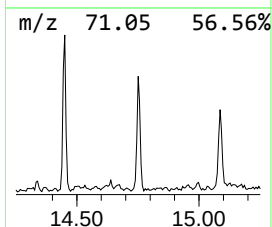
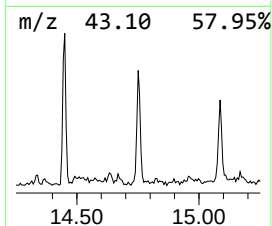
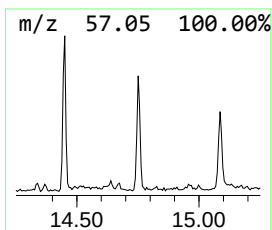
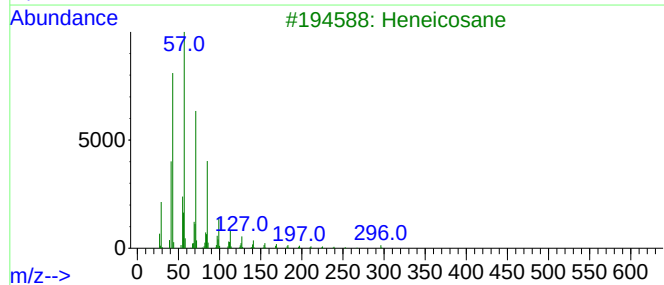
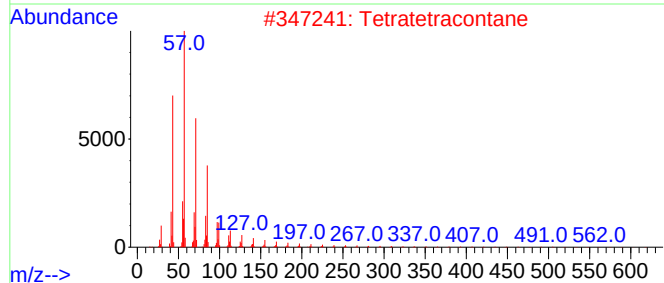
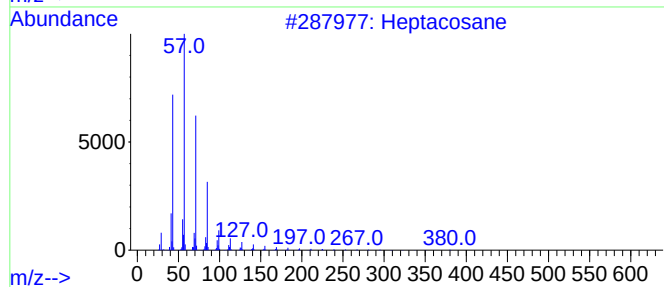
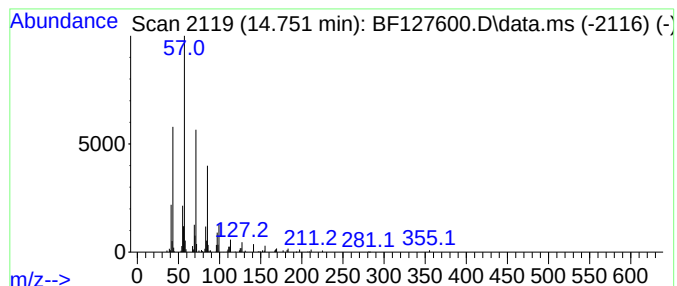
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	2.88 ng	99403	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Pentadecane	212	C15H32	000629-62-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

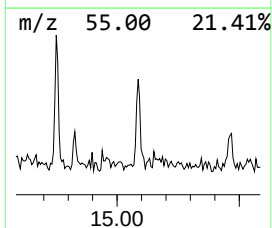
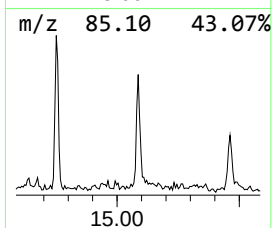
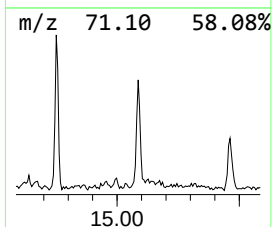
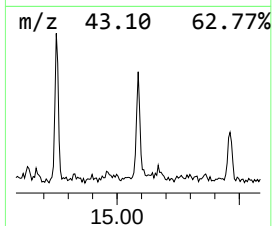
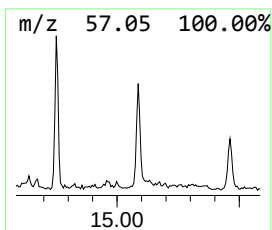
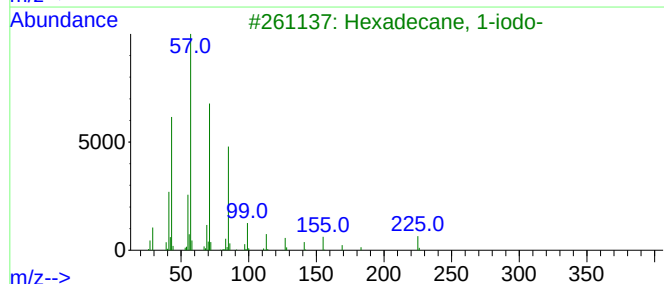
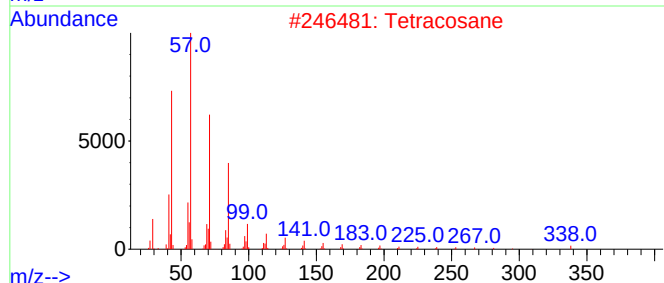
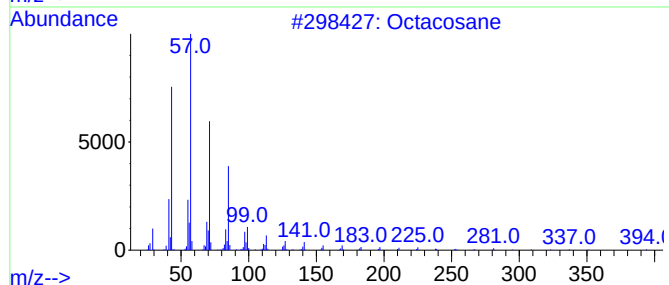
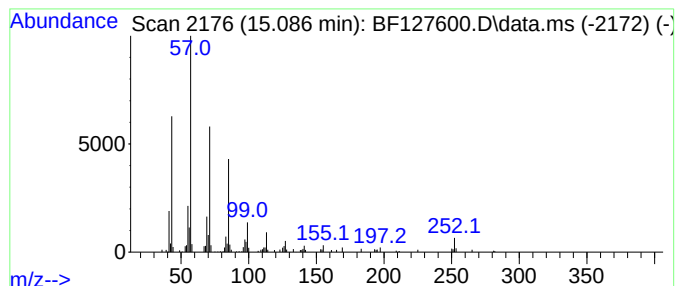
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	2.53 ng	82990	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Tetracosane	338	C24H50	000646-31-1	87
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

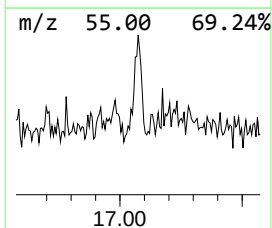
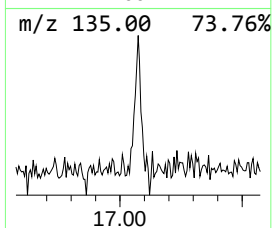
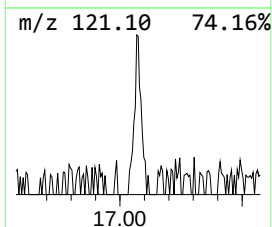
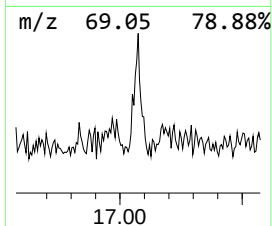
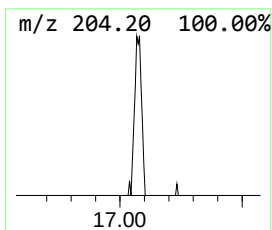
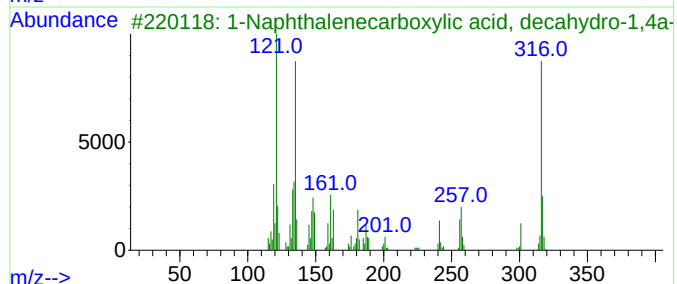
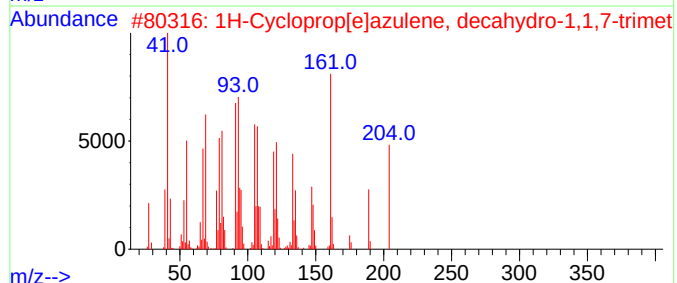
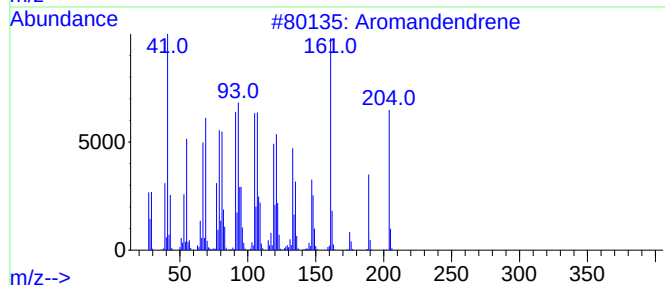
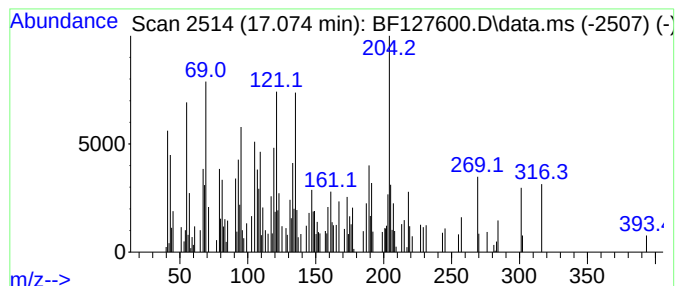
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Aromandendrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.074	3.06 ng	100156	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aromandendrene	204	C15H24	000489-39-4	64
2			1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	50
3			1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	50
4			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	45
5			1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127600.D
Acq On : 31 Mar 2022 13:11
Operator : CG\JU
Sample : N2171-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSE-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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-...	5.075	3.0	ng	77702	1	6.834	512676	20.0
Hexatriacontane	13.827	4.7	ng	163079	5	14.015	690424	20.0
Eicosane	14.145	3.5	ng	121197	5	14.015	690424	20.0
Octacosane	14.451	3.5	ng	119411	5	14.015	690424	20.0
Heptacosane	14.751	2.9	ng	99403	5	14.015	690424	20.0
Tetracosane	15.086	2.5	ng	82990	6	15.498	655506	20.0
Aromandendrene	17.074	3.1	ng	100156	6	15.498	655506	20.0