

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
 Data File : BM028146.D
 Acq On : 17 Dec 2020 18:09
 Operator : JU/CG
 Sample : L5036-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-5

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_M\Methods\8270-BM121620.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028146.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.375	27	32	45	rVB	98273	150785	2.50%	0.473%
2	5.704	421	428	437	rBV	1520831	2212174	36.74%	6.945%
3	7.345	699	707	723	rBV	1542717	2543942	42.25%	7.986%
4	7.792	778	783	792	rBV	108906	174590	2.90%	0.548%
5	8.210	843	854	860	rBV	469310	742759	12.34%	2.332%
6	9.386	1046	1054	1061	rBV	1034324	1714999	28.49%	5.384%
7	11.039	1328	1335	1341	rVB	609823	1008657	16.75%	3.166%
8	13.463	1738	1747	1755	rBV	2503901	3597645	59.76%	11.294%
9	13.716	1785	1790	1799	rVB	79173	118529	1.97%	0.372%
10	14.280	1879	1886	1893	rBV	339673	487331	8.09%	1.530%
11	14.833	1970	1980	1988	rBV	905433	1339293	22.25%	4.204%
12	16.304	2224	2230	2243	rBV	1763496	2444414	40.60%	7.674%
13	17.556	2436	2443	2447	rBV	1151056	1684961	27.99%	5.290%
14	17.598	2447	2450	2456	rVB	106084	143700	2.39%	0.451%
15	18.409	2583	2588	2594	rBV2	197976	332123	5.52%	1.043%
16	18.462	2594	2597	2606	rVB2	54888	101127	1.68%	0.317%
17	19.580	2778	2787	2792	rBV	171082	259849	4.32%	0.816%
18	19.668	2797	2802	2814	rBV	166720	293401	4.87%	0.921%
19	19.898	2837	2841	2844	rBV3	34852	62039	1.03%	0.195%
20	19.939	2844	2848	2853	rVB	159952	204903	3.40%	0.643%
21	20.127	2874	2880	2885	rBV	4929466	6020561	100.00%	18.900%
22	20.421	2927	2930	2935	rVB3	54601	70275	1.17%	0.221%
23	21.356	3085	3089	3100	rBV	449277	728790	12.11%	2.288%
24	21.668	3136	3142	3146	rBV	1884037	2490025	41.36%	7.817%
25	21.703	3146	3148	3154	rVB	123759	152507	2.53%	0.479%
26	22.874	3343	3347	3352	rVB	280102	371083	6.16%	1.165%
27	24.038	3538	3545	3560	rVB	1169150	2403699	39.92%	7.546%

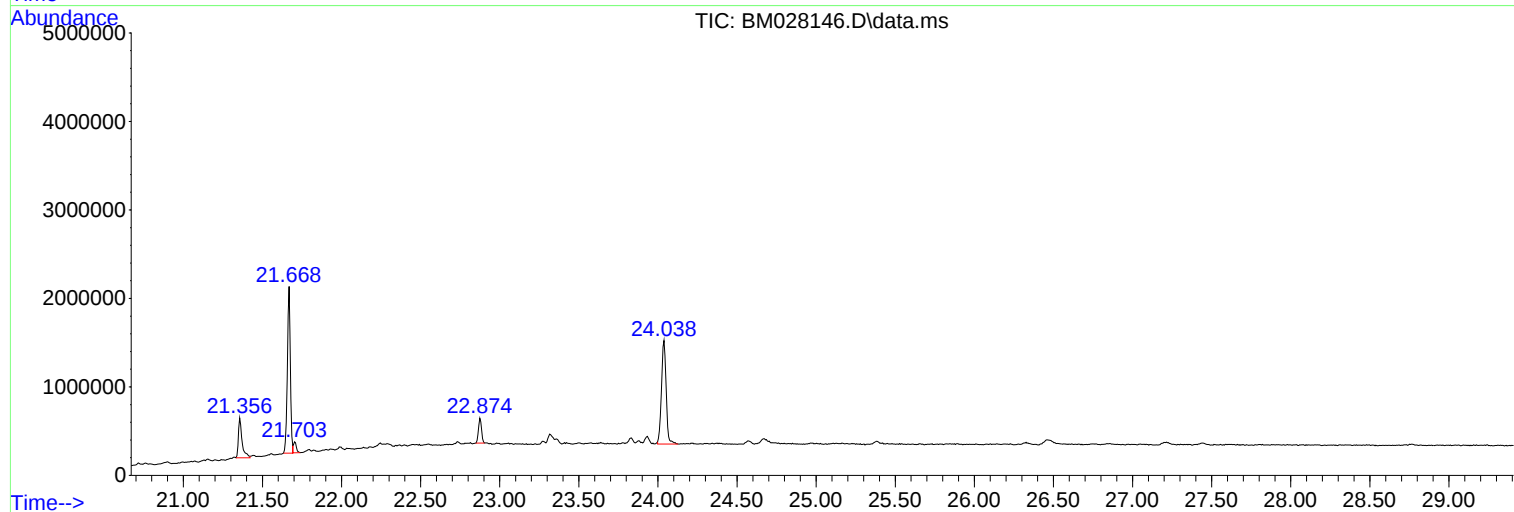
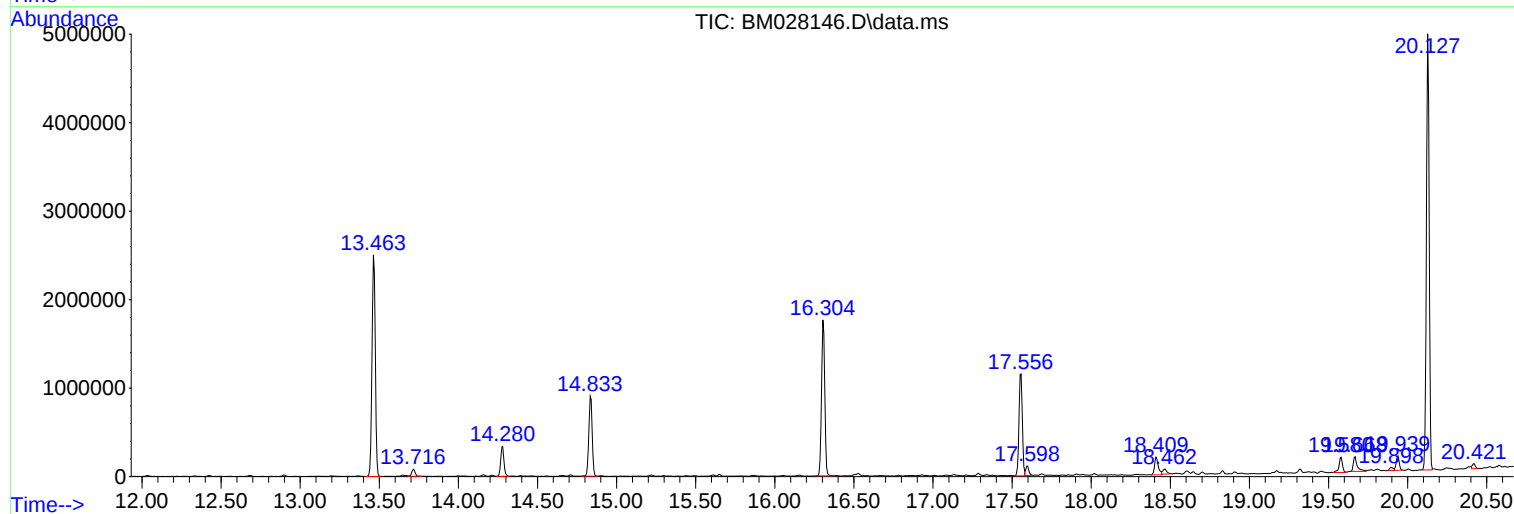
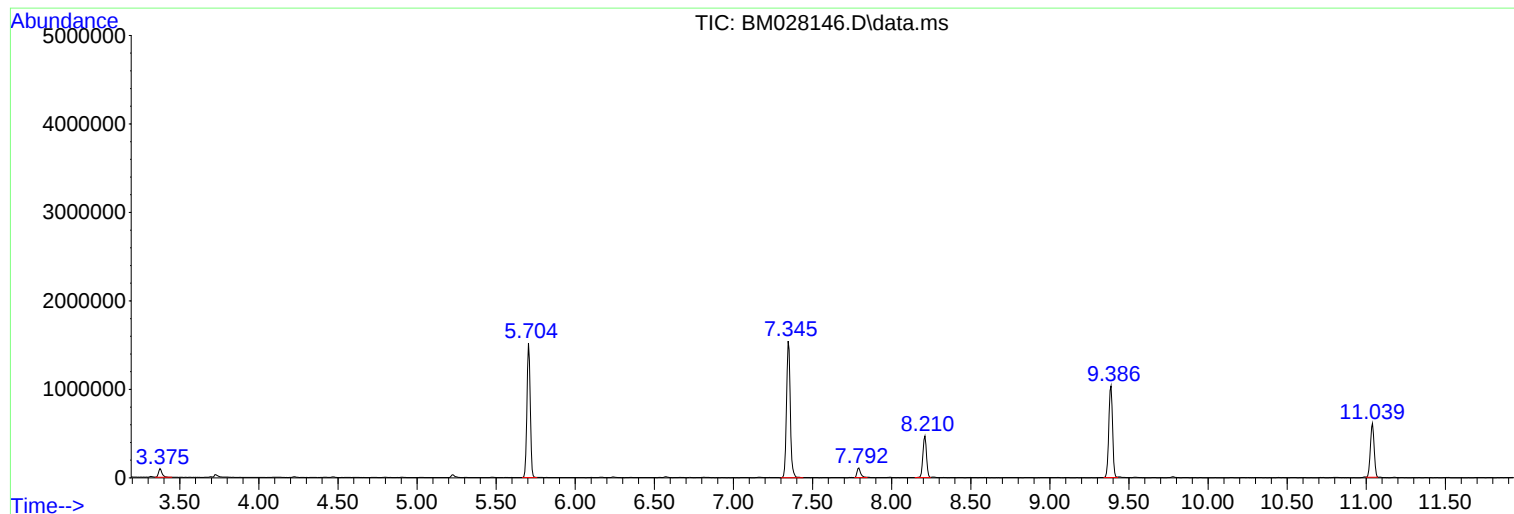
Sum of corrected areas: 31854161

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-5

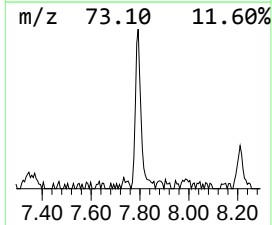
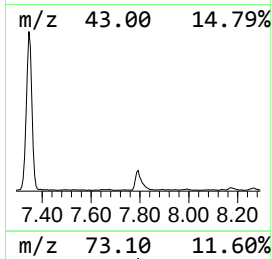
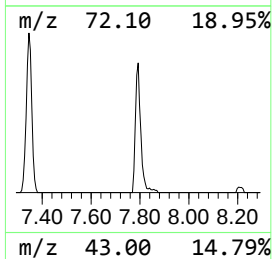
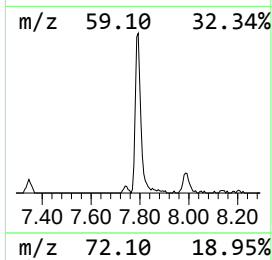
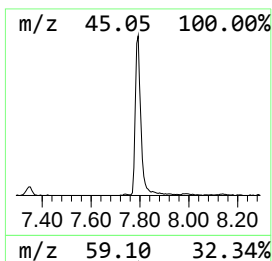
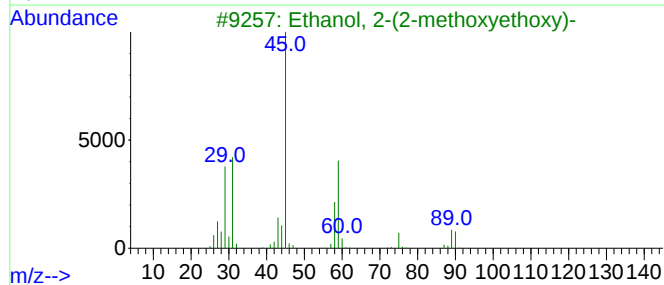
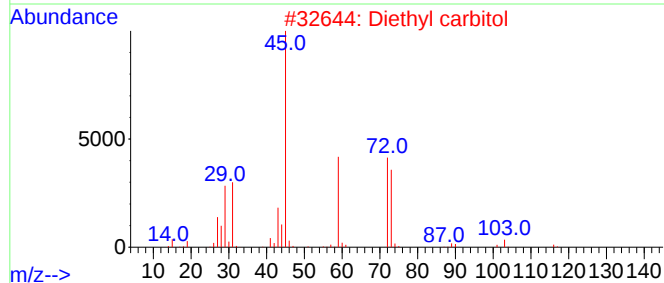
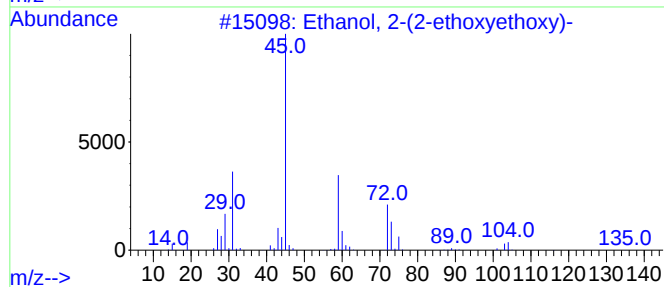
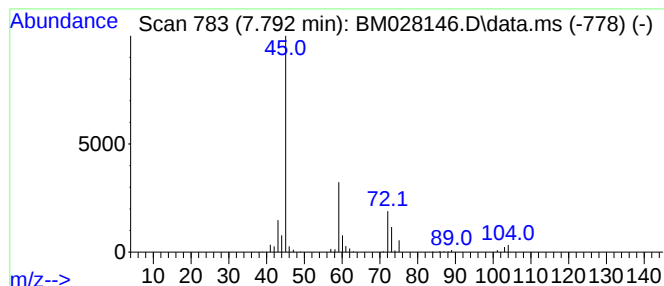
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.792	4.70 ng	174590	1,4-Dichlorobenzene-d4	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	78
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	64
4			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	50
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-5

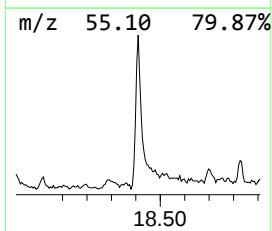
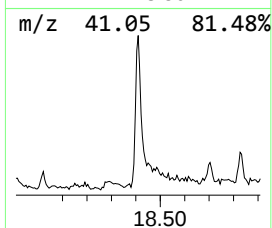
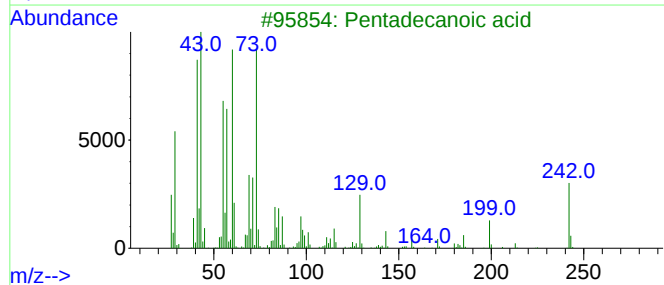
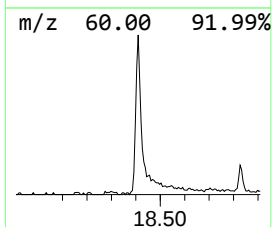
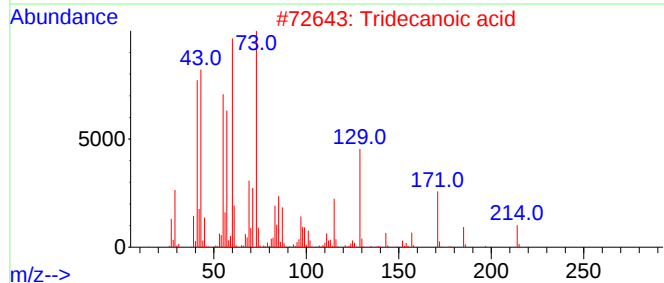
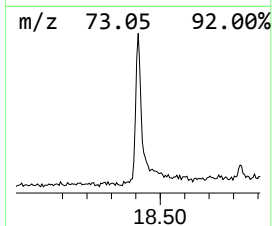
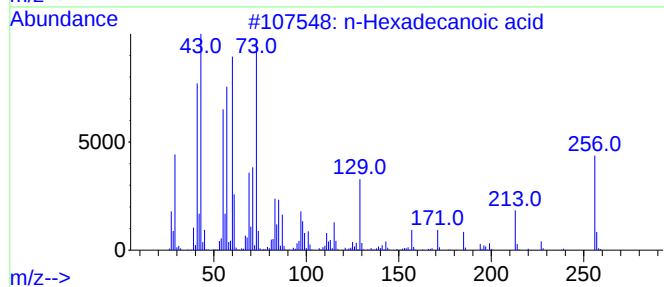
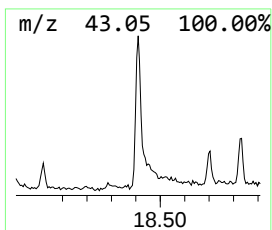
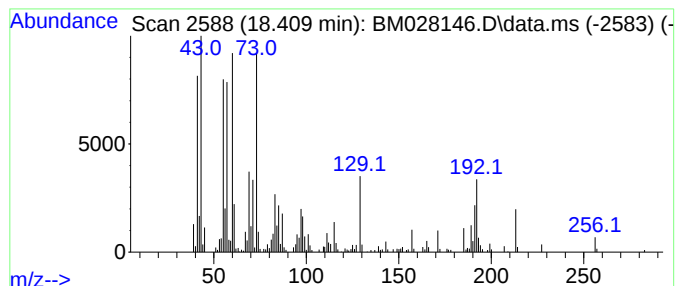
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.409	3.94 ng	332123	Phenanthrene-d10	17.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampled :
B-5

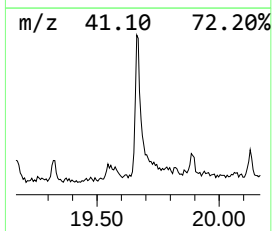
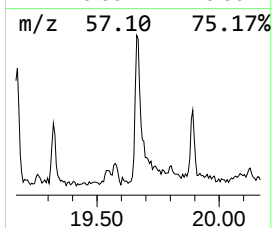
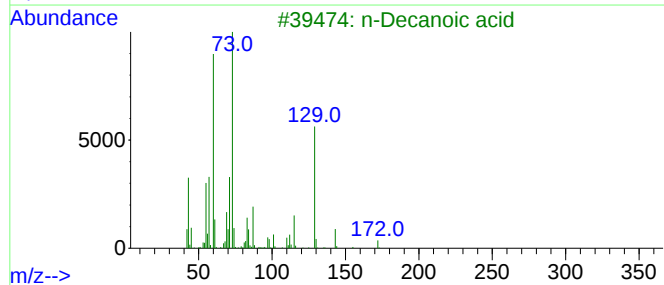
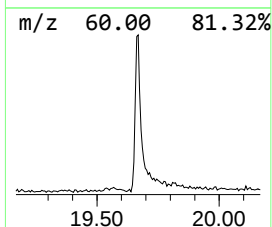
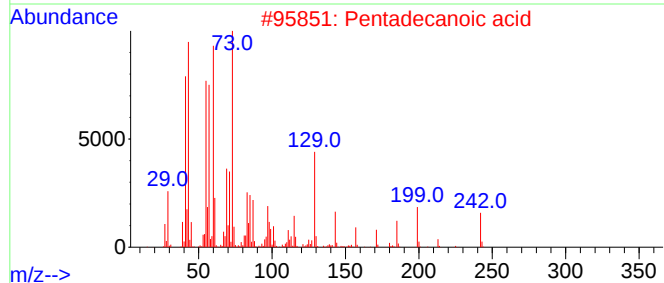
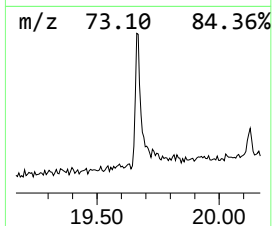
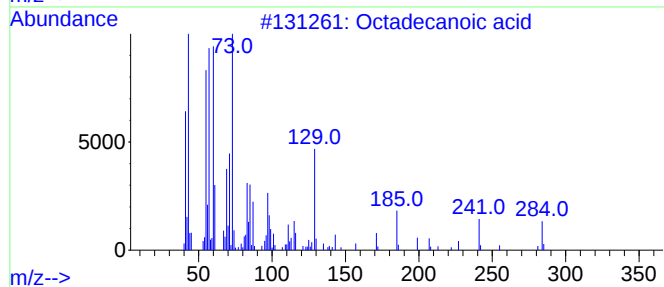
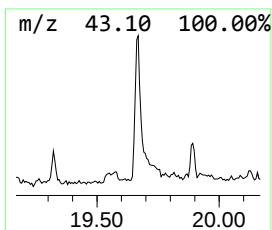
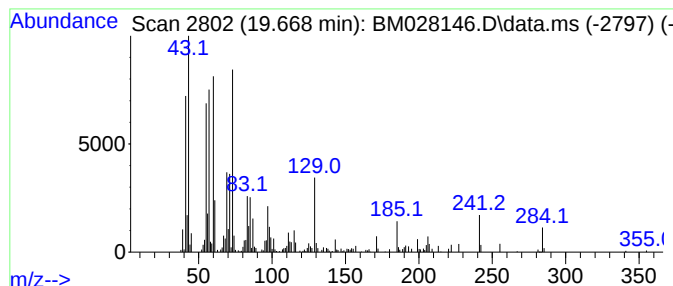
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.668	2.36 ng	293401	Chrysene-d12	21.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Decanoic acid	172	C10H20O2	000334-48-5	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-5

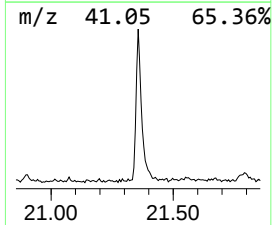
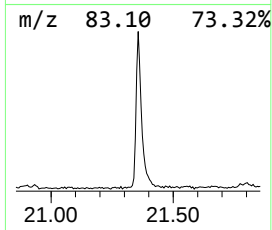
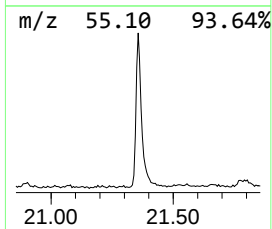
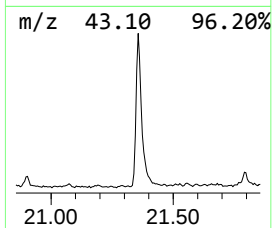
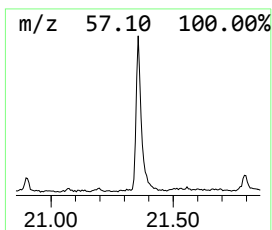
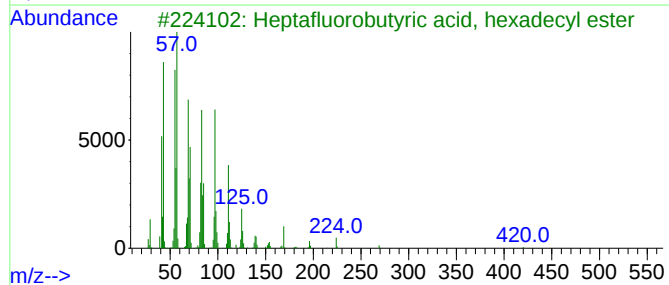
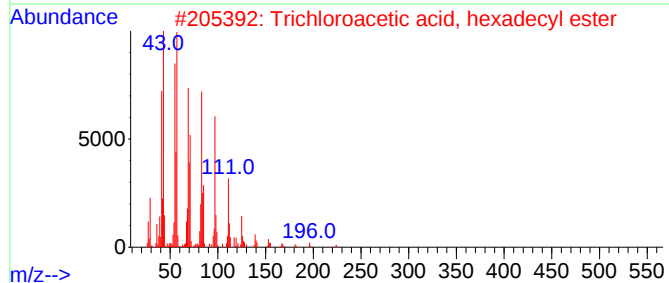
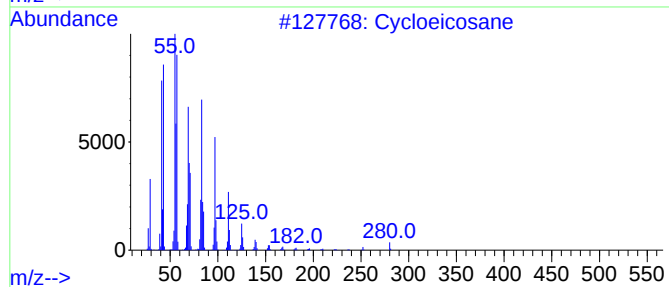
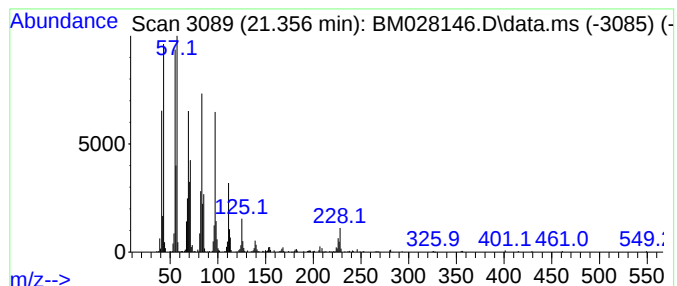
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cycloeicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.356	5.85 ng	728790	Chrysene-d12	21.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	96
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-5

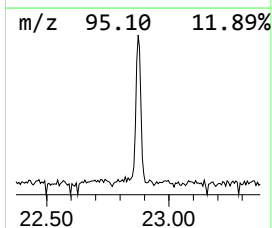
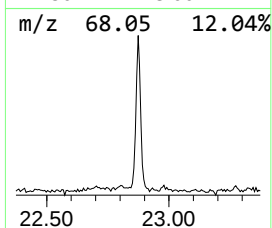
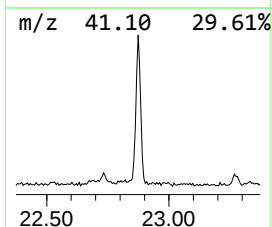
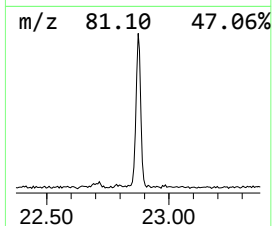
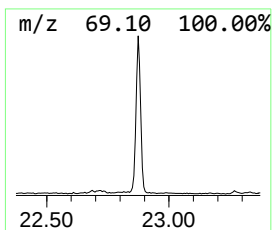
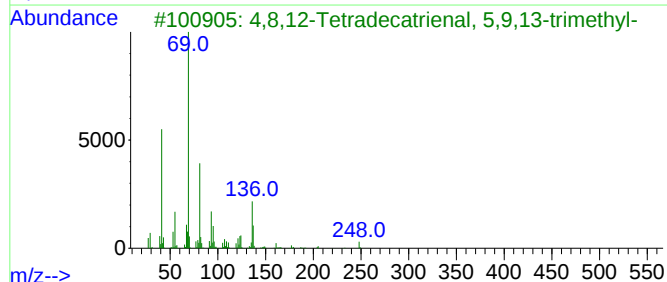
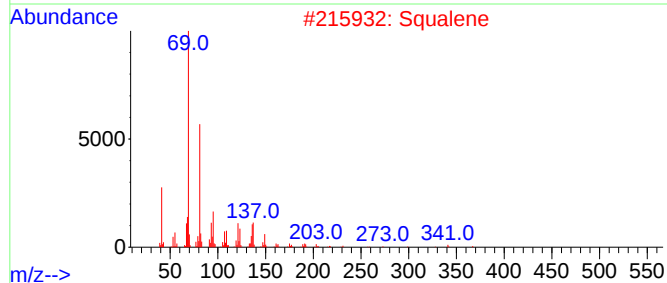
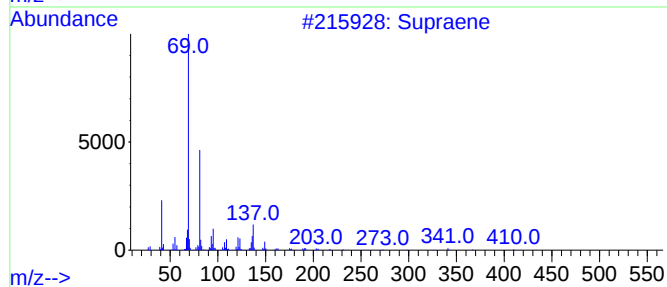
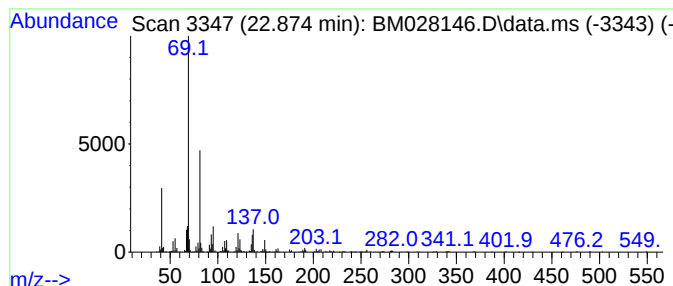
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.874	3.09 ng	371083	Perylene-d12	24.038

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			Squalene	410	C30H50	000111-02-4	87
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64
5			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121720\
Data File : BM028146.D
Acq On : 17 Dec 2020 18:09
Operator : JU/CG
Sample : L5036-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-e...	7.792	4.7	ng	174590	1	8.210	742759	20.0
n-Hexadecanoic ...	18.409	3.9	ng	332123	4	17.557	1684960	20.0
Octadecanoic acid	19.668	2.4	ng	293401	5	21.668	2490030	20.0
Cycloeicosane	21.356	5.8	ng	728790	5	21.668	2490030	20.0
Supraene	22.874	3.1	ng	371083	6	24.038	2403700	20.0