

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
 Data File : BM033506.D
 Acq On : 17 Dec 2021 15:12
 Operator : CG/JU
 Sample : M5064-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SASP2-121-1-(5-10)

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-BM121621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.037	301	306	319	rBV	262386	395323	15.44%	2.731%
2	5.502	379	385	398	rBV	979613	1464790	57.20%	10.121%
3	6.125	485	491	497	rBV	27142	40277	1.57%	0.278%
4	7.113	651	659	673	rBV	952265	1611856	62.95%	11.137%
5	7.937	790	799	806	rBV	234997	371513	14.51%	2.567%
6	9.113	990	999	1010	rBV	612790	1069505	41.77%	7.390%
7	10.548	1237	1243	1254	rBV2	10993	27078	1.06%	0.187%
8	10.748	1270	1277	1288	rBV	292943	499623	19.51%	3.452%
9	13.207	1688	1695	1703	rBV	1518911	2254051	88.03%	15.574%
10	13.401	1723	1728	1737	rVB2	14776	25980	1.01%	0.180%
11	14.583	1923	1929	1937	rBV	444491	647061	25.27%	4.471%
12	16.071	2172	2182	2196	rBV	1093624	1635454	63.87%	11.300%
13	17.330	2390	2396	2404	rBV	495325	723131	28.24%	4.996%
14	18.218	2543	2547	2553	rBV	64383	94166	3.68%	0.651%
15	19.495	2761	2764	2769	rBV6	21353	28713	1.12%	0.198%
16	19.954	2836	2842	2850	rBV	2083619	2560625	100.00%	17.693%
17	21.212	3052	3056	3062	rBV	139874	177766	6.94%	1.228%
18	21.512	3102	3107	3112	rBV	340007	460078	17.97%	3.179%
19	23.924	3512	3517	3526	rVB2	180639	385825	15.07%	2.666%

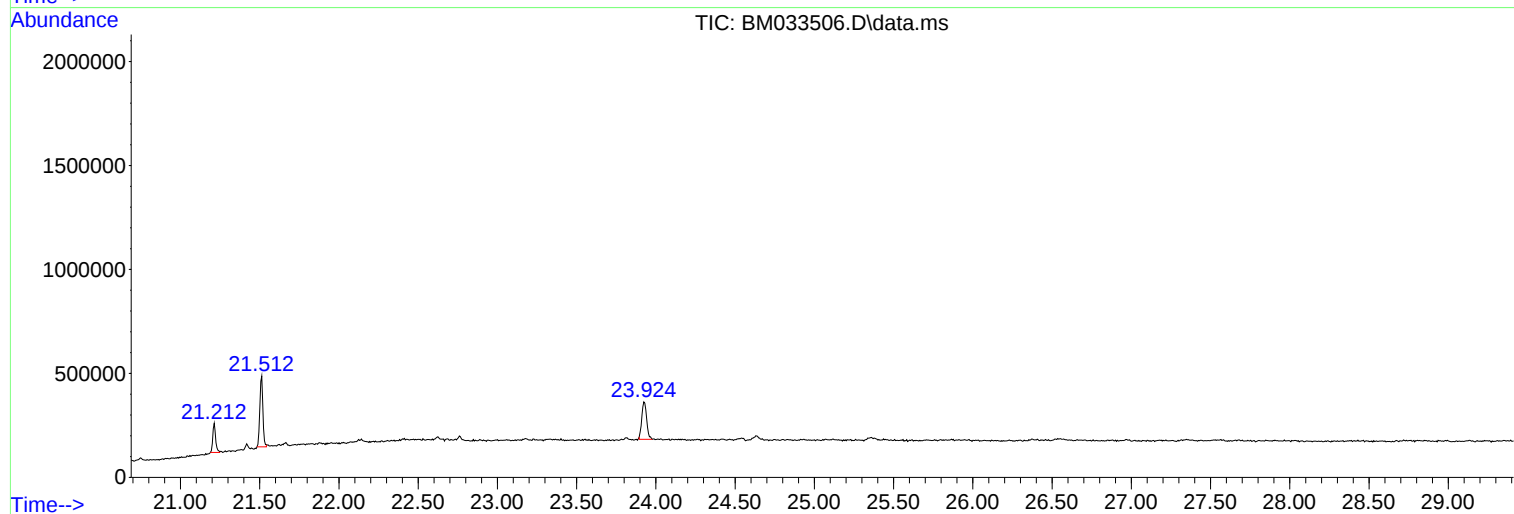
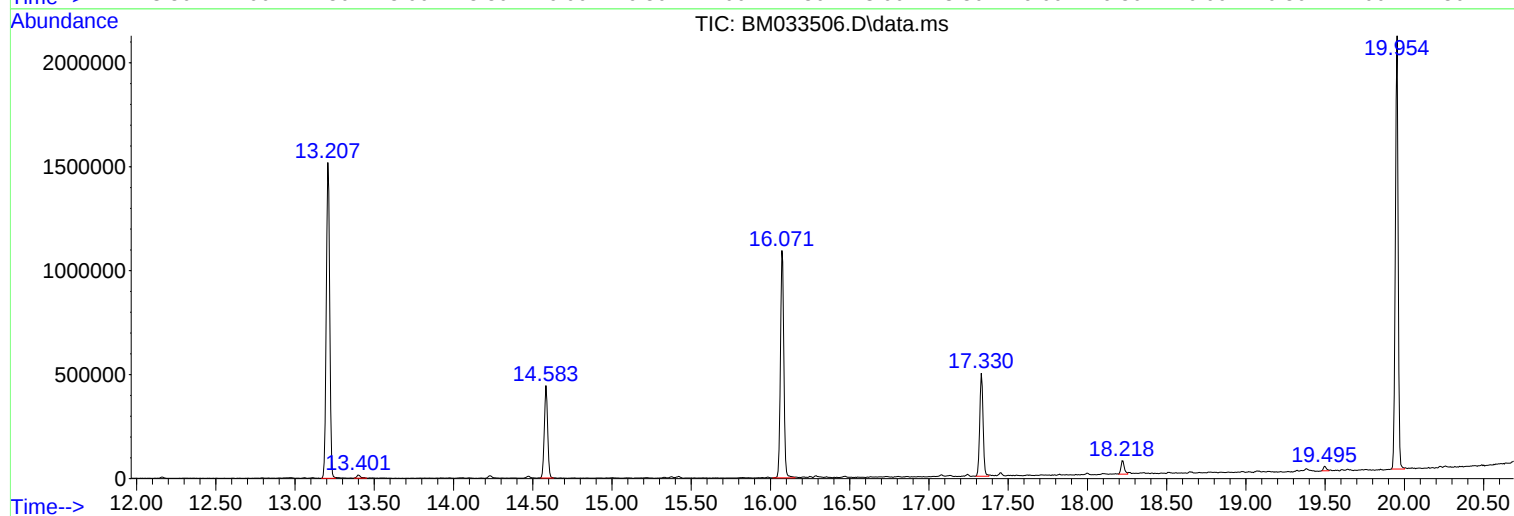
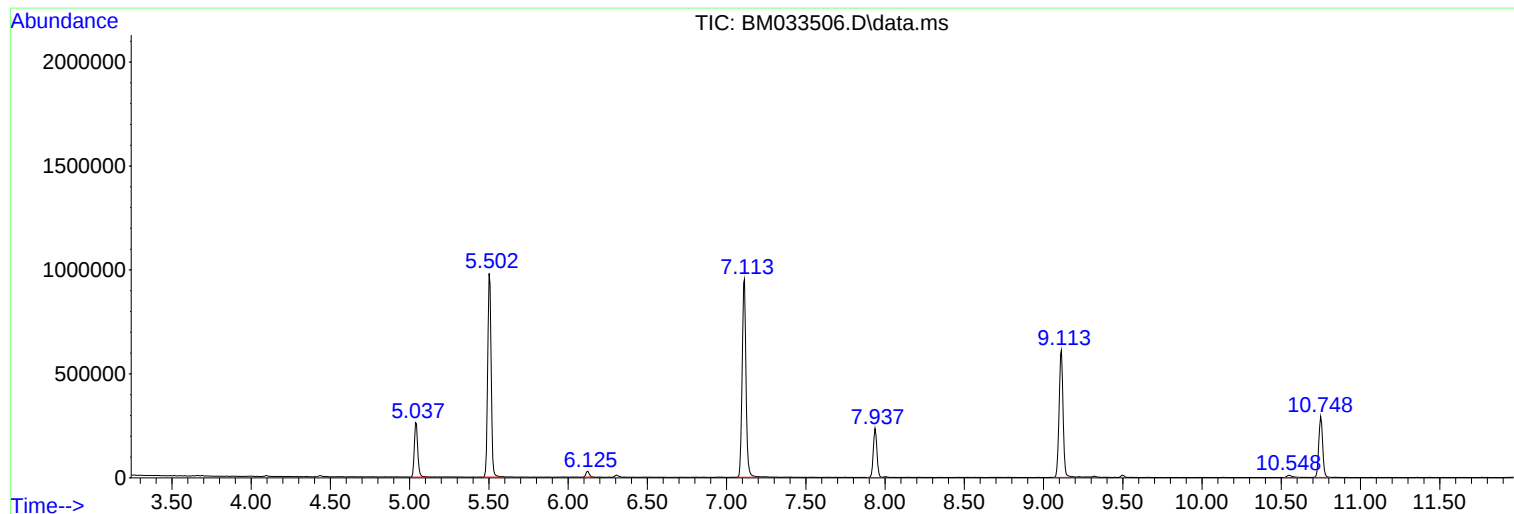
Sum of corrected areas: 14472815

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033506.D
Acq On : 17 Dec 2021 15:12
Operator : CG/JU
Sample : M5064-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-121-1-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.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_M\Data\BM121721\
Data File : BM033506.D
Acq On : 17 Dec 2021 15:12
Operator : CG/JU
Sample : M5064-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-121-1-(5-10)

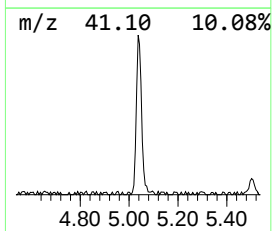
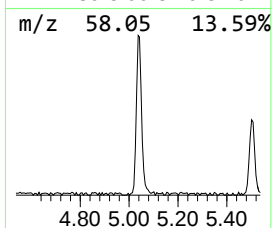
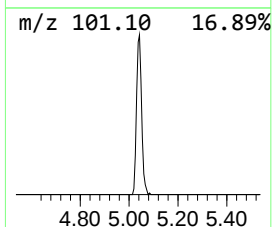
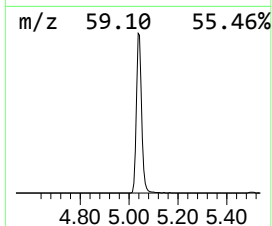
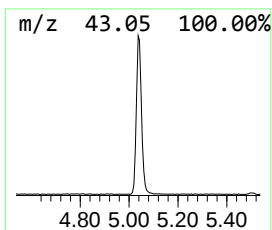
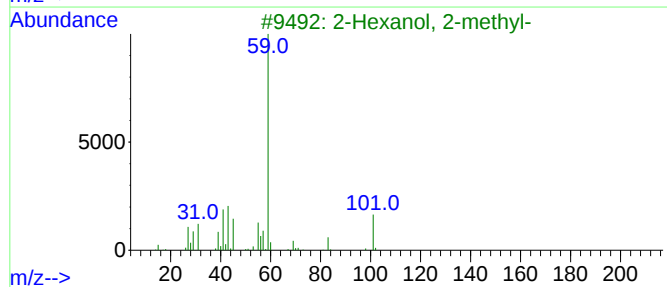
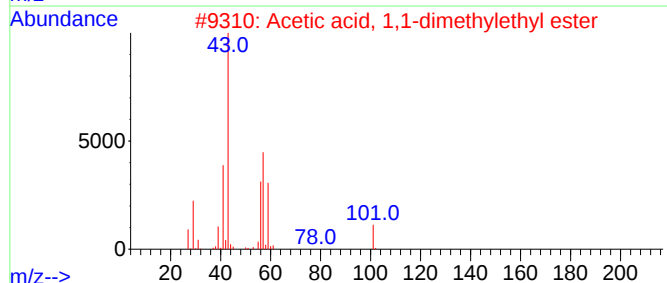
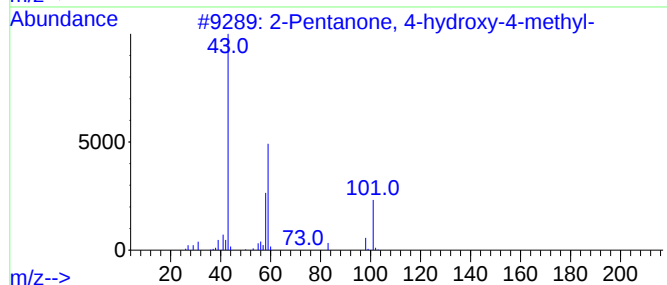
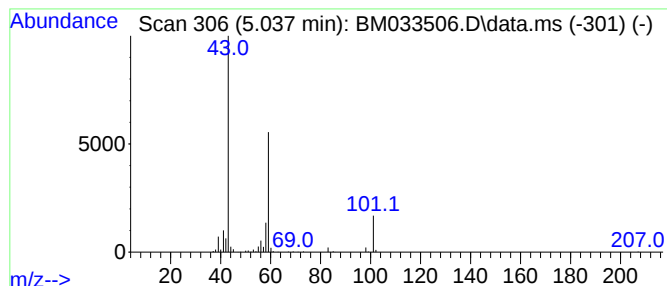
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.037	21.28 ng	395323	1,4-Dichlorobenzene-d4	7.937

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033506.D
Acq On : 17 Dec 2021 15:12
Operator : CG/JU
Sample : M5064-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-121-1-(5-10)

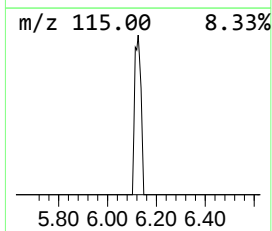
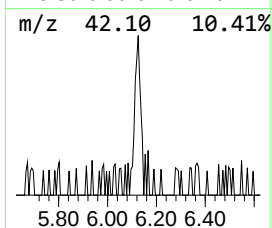
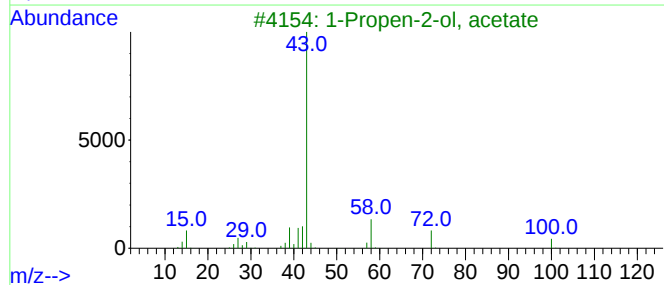
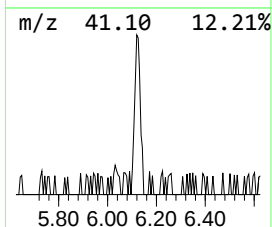
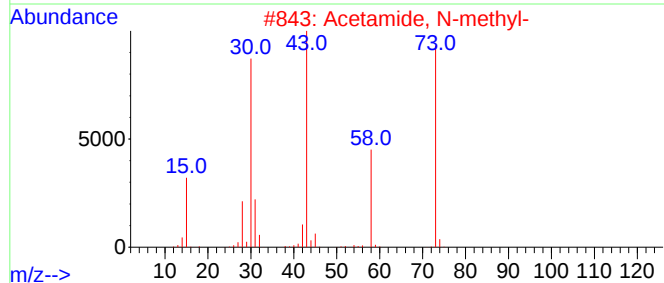
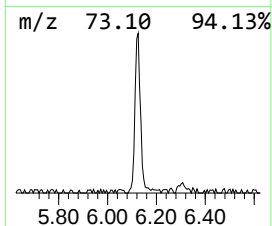
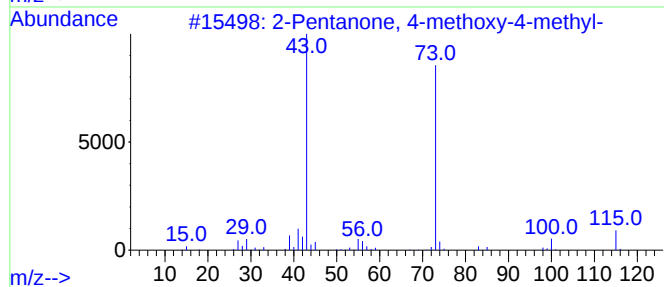
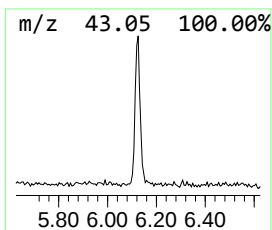
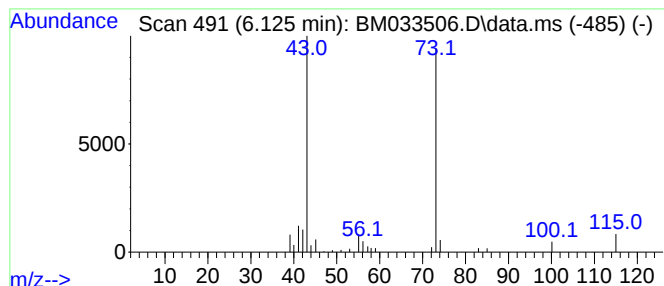
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.125	2.17 ng	40277	1,4-Dichlorobenzene-d4	7.937

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	64
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	17
4		2-Heptanone	114	C7H14O	000110-43-0	17
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033506.D
Acq On : 17 Dec 2021 15:12
Operator : CG/JU
Sample : M5064-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-121-1-(5-10)

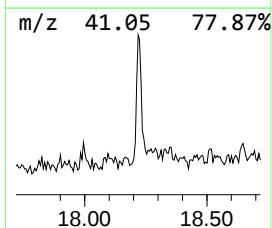
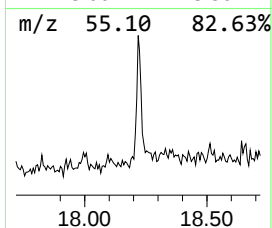
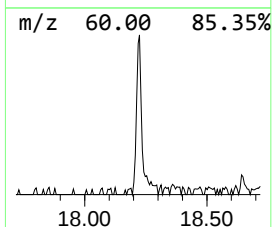
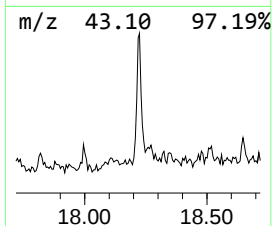
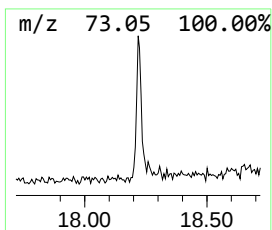
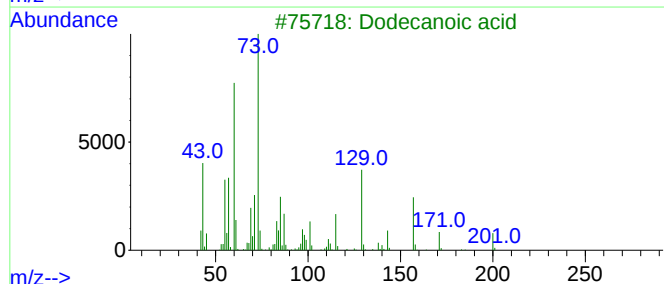
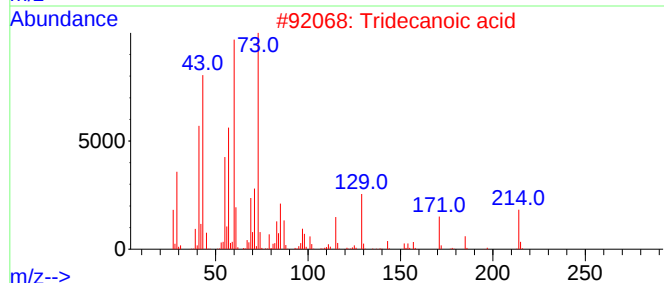
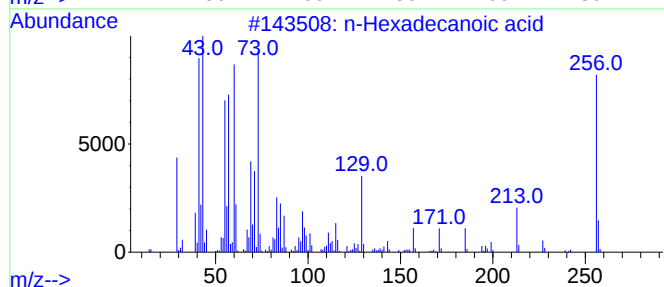
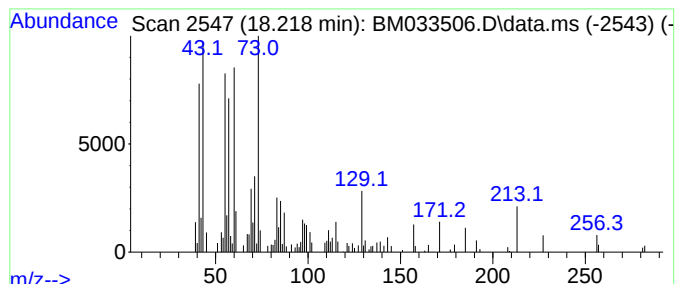
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	2.60 ng	94166	Phenanthrene-d10	17.330

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	74
3			Dodecanoic acid	200	C12H24O2	000143-07-7	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033506.D
Acq On : 17 Dec 2021 15:12
Operator : CG/JU
Sample : M5064-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-121-1-(5-10)

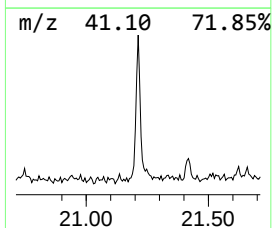
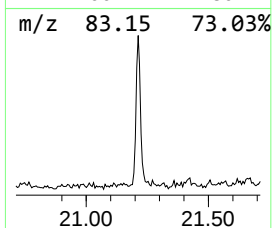
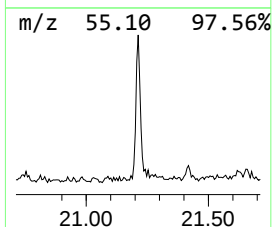
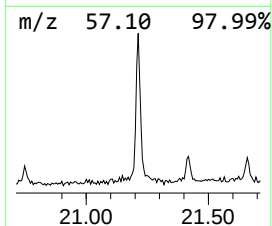
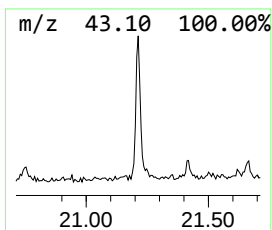
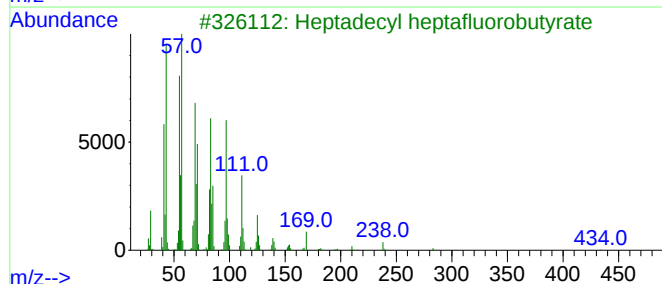
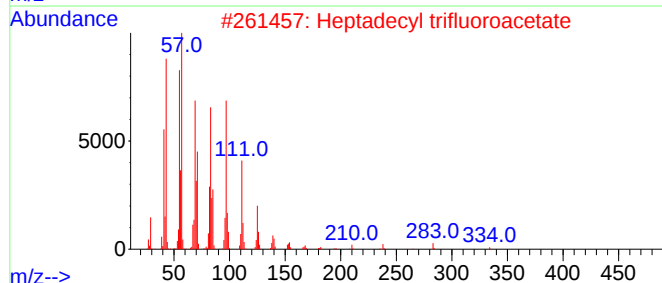
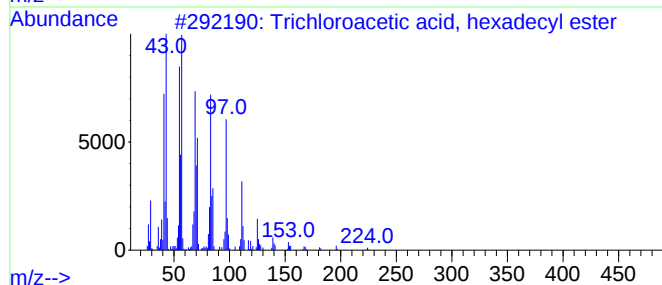
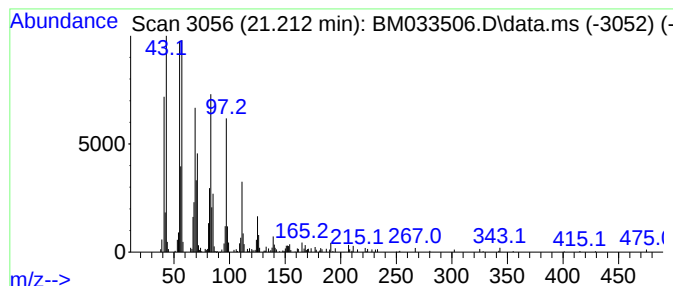
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.212	7.73 ng	177766	Chrysene-d12	21.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033506.D
Acq On : 17 Dec 2021 15:12
Operator : CG/JU
Sample : M5064-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-121-1-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.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-...	5.037	21.3	ng	395323	1	7.937	371513	20.0
2-Pentanone, 4-...	6.125	2.2	ng	40277	1	7.937	371513	20.0
n-Hexadecanoic ...	18.218	2.6	ng	94166	4	17.330	723131	20.0
Trichloroacetic...	21.212	7.7	ng	177766	5	21.512	460078	20.0