

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
 Data File : BM039982.D
 Acq On : 24 May 2023 13:56
 Operator : CG/JU
 Sample : 02868-21
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP17

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-BM052323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.722	61	74	78	rBV	338083	871646	7.29%	0.862%
2	4.216	120	158	160	rBV	1408347	8698097	72.73%	8.603%
3	4.869	257	269	274	rBV	319559	679105	5.68%	0.672%
4	5.004	283	292	296	rBV	189050	334192	2.79%	0.331%
5	5.098	302	308	313	rBV	261569	358832	3.00%	0.355%
6	5.563	375	387	398	rBV	4822529	6751052	56.45%	6.677%
7	7.169	652	660	674	rBV	4323503	6651924	55.62%	6.579%
8	8.016	797	804	812	rBV	1299566	1981401	16.57%	1.960%
9	9.180	994	1002	1010	rBV	2438486	3915033	32.74%	3.872%
10	10.045	1138	1149	1156	rBV	133695	260506	2.18%	0.258%
11	10.833	1276	1283	1289	rBV	1577335	2597573	21.72%	2.569%
12	11.351	1361	1371	1384	rBV	176582	334445	2.80%	0.331%
13	12.610	1579	1585	1593	rBV2	214832	415110	3.47%	0.411%
14	13.280	1692	1699	1706	rBV	6090736	8483609	70.94%	8.391%
15	13.980	1813	1818	1824	rBV	267967	384480	3.21%	0.380%
16	14.651	1927	1932	1941	rVB	2050718	2956831	24.72%	2.924%
17	15.462	2061	2070	2077	rBV3	55122	130720	1.09%	0.129%
18	16.004	2152	2162	2171	rVB	972174	1420818	11.88%	1.405%
19	16.133	2178	2184	2191	rBV	4817505	6636941	55.50%	6.564%
20	16.568	2254	2258	2263	rBV	169063	224589	1.88%	0.222%
21	17.392	2393	2398	2404	rBV	2236333	3203898	26.79%	3.169%
22	17.798	2461	2467	2474	rVB	83865	141181	1.18%	0.140%
23	18.292	2545	2551	2559	rBV	2103931	3027038	25.31%	2.994%
24	18.362	2560	2563	2571	rVB	229071	353021	2.95%	0.349%
25	18.809	2635	2639	2647	rBV	114181	161485	1.35%	0.160%
26	19.444	2743	2747	2761	rVB2	306025	566561	4.74%	0.560%
27	19.562	2762	2767	2784	rBV	1505080	2322424	19.42%	2.297%
28	19.780	2800	2804	2806	rBV	148393	218084	1.82%	0.216%
29	19.809	2806	2809	2819	rVB	296155	476372	3.98%	0.471%
30	20.009	2838	2843	2849	rBV	10026699	11959249	100.00%	11.828%
31	20.615	2935	2946	2958	rVB3	1274151	5241665	43.83%	5.184%
32	20.815	2970	2980	2989	rBV3	929311	3552273	29.70%	3.513%
33	21.115	3028	3031	3035	rVB	489281	533851	4.46%	0.528%
34	21.274	3055	3058	3065	rVB2	914106	1125785	9.41%	1.113%
35	21.486	3090	3094	3098	rVB	434859	512335	4.28%	0.507%
36	21.574	3102	3109	3113	rVV	3094552	4761133	39.81%	4.709%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

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-BM052323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.609	3113	3115	3121	rVB	513690	592381	4.95%	0.586%
38	21.691	3126	3129	3133	rVV	291572	394033	3.29%	0.390%
39	21.733	3133	3136	3145	rVB	259439	380818	3.18%	0.377%
40	22.203	3213	3216	3222	rBV3	241738	373099	3.12%	0.369%
41	22.427	3251	3254	3260	rBV	207923	262916	2.20%	0.260%
42	22.715	3300	3303	3313	rVB2	189683	276370	2.31%	0.273%
43	23.280	3394	3399	3403	rBV2	590862	1030483	8.62%	1.019%
44	24.021	3519	3525	3537	rVB	1943089	3922863	32.80%	3.880%
45	24.674	3631	3636	3647	rVB2	601838	1629800	13.63%	1.612%

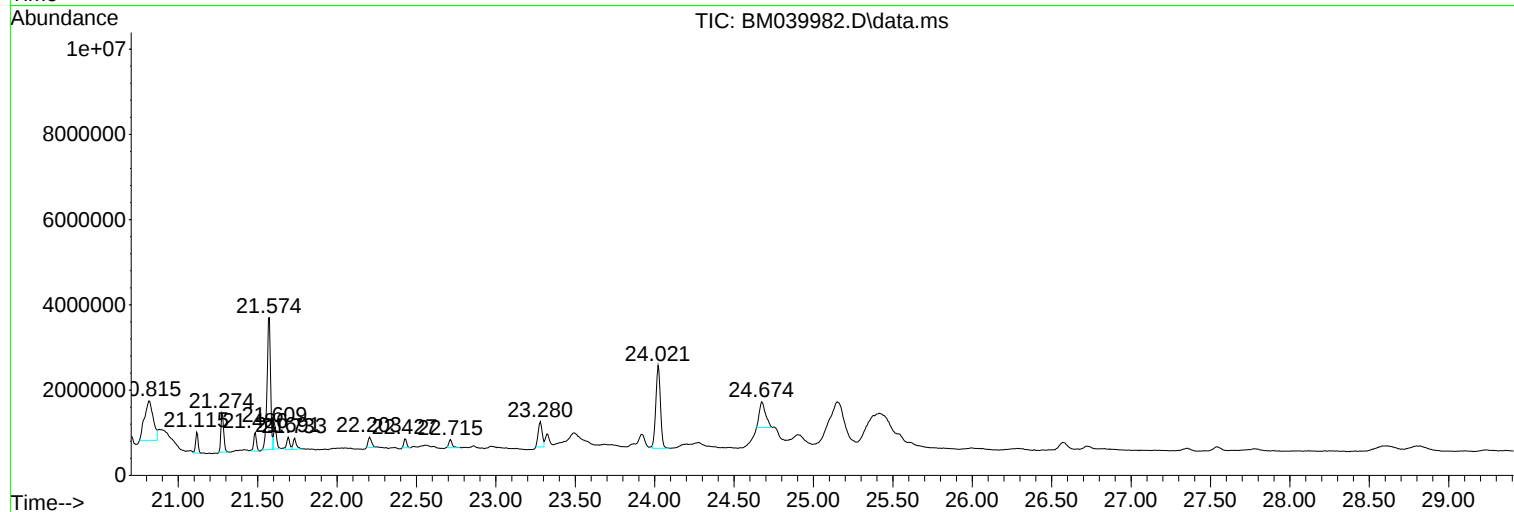
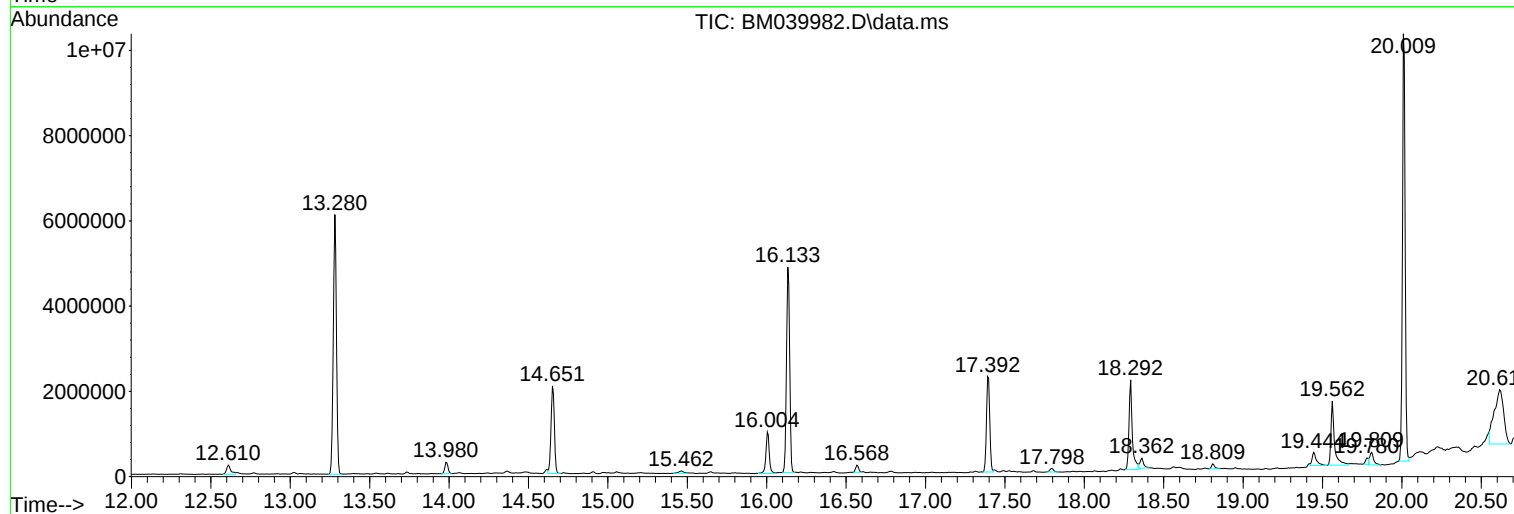
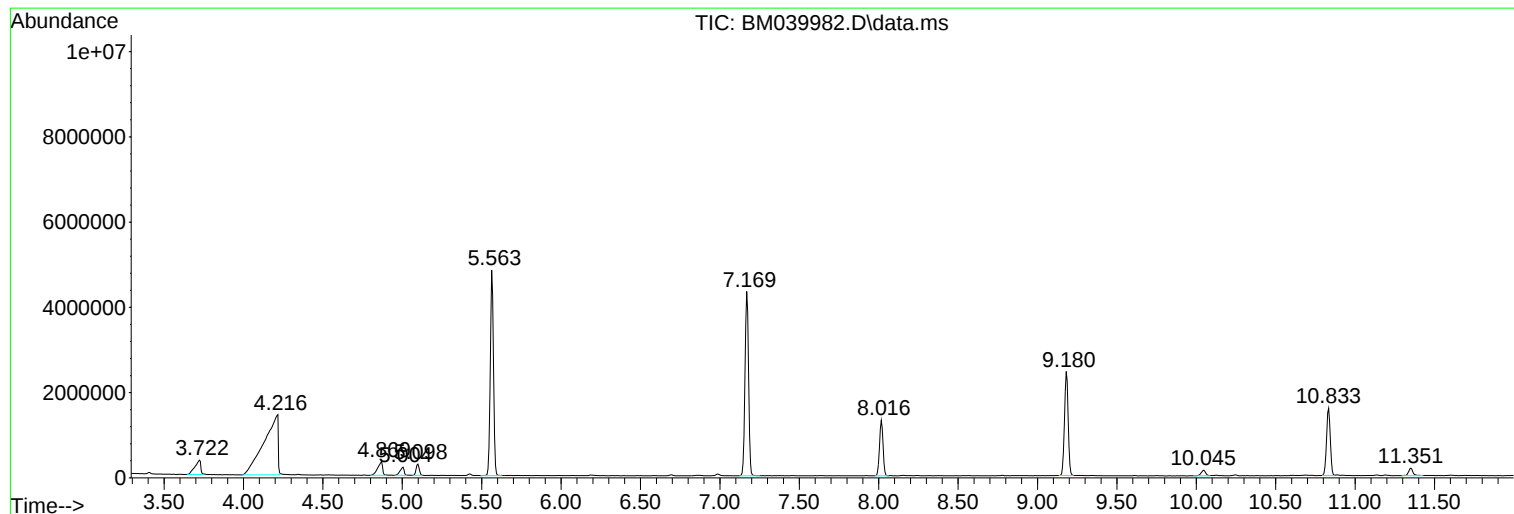
Sum of corrected areas: 101106022

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

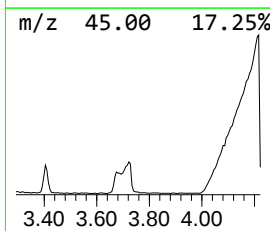
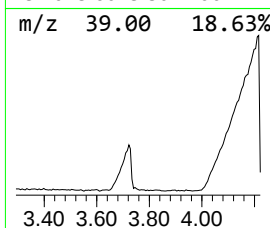
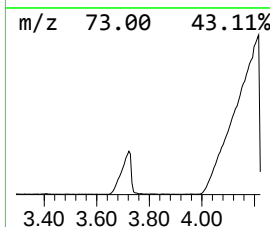
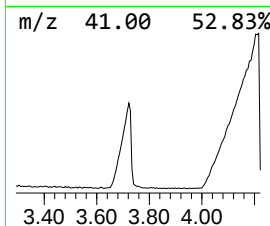
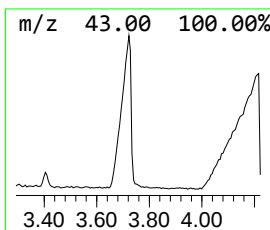
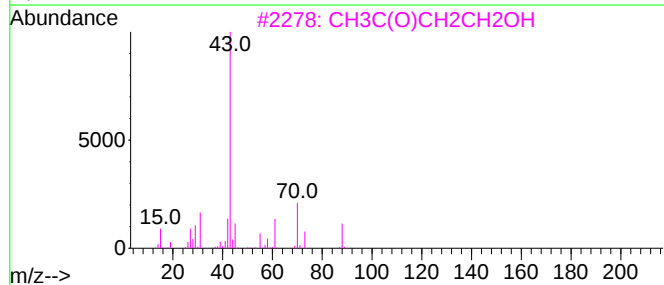
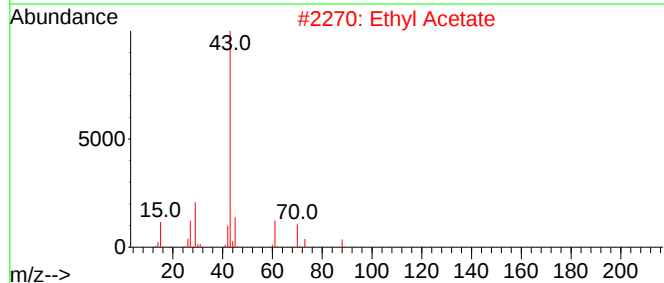
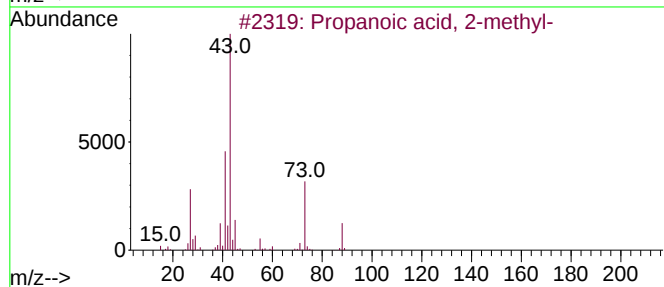
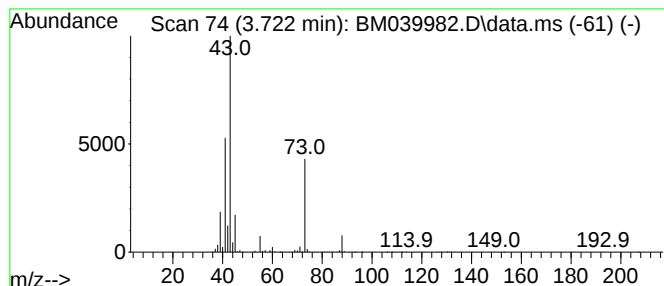
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.722	8.80 ng	871646	1,4-Dichlorobenzene-d4	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	50
3		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	45
4		Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	37
5		Methyl glyoxal	72	C3H4O2	000078-98-8	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

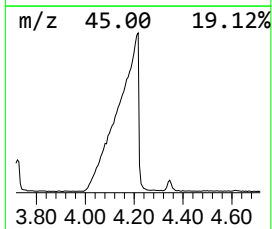
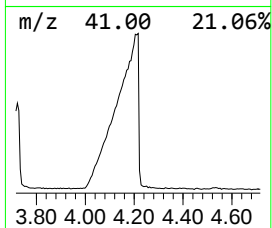
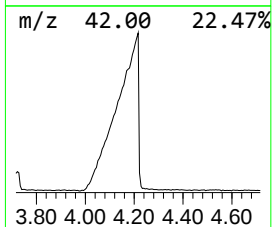
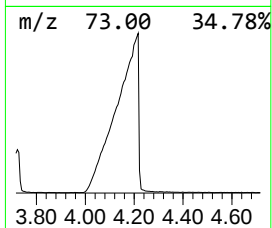
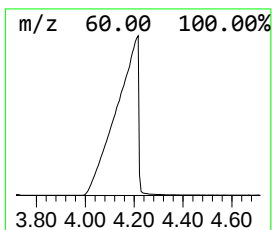
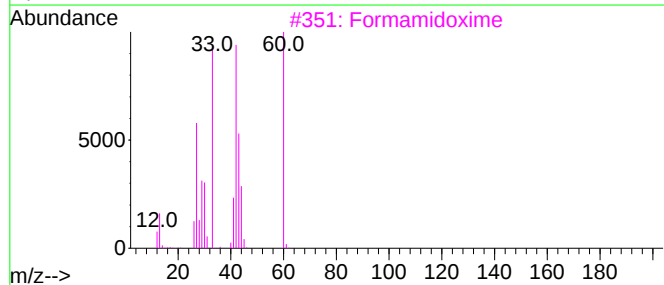
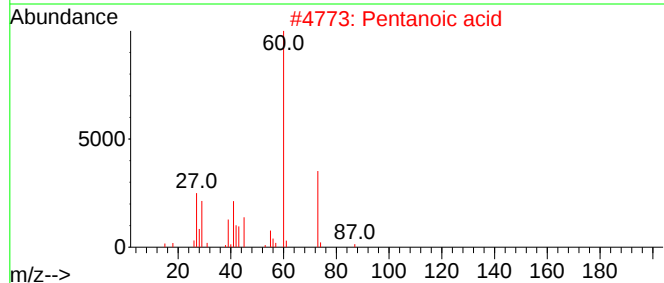
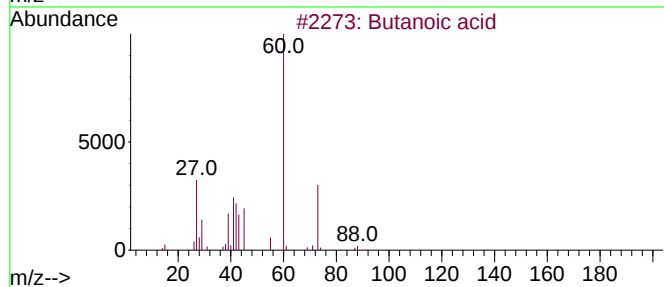
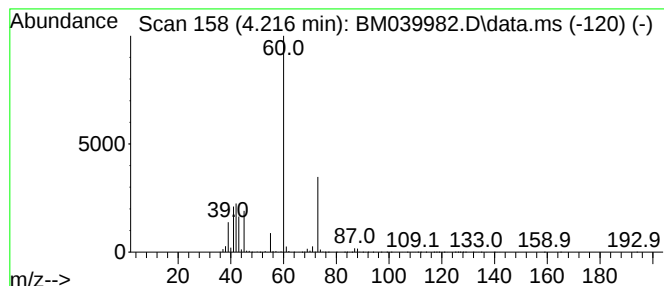
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.216	87.80 ng	8698100	1,4-Dichlorobenzene-d4	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	91
2			Pentanoic acid	102	C5H10O2	000109-52-4	39
3			Formamidoxime	60	CH4N2O	000624-82-8	9
4			Hexanoic acid	116	C6H12O2	000142-62-1	9
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

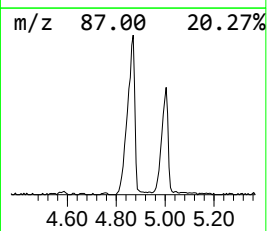
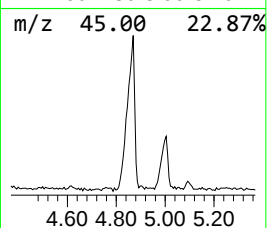
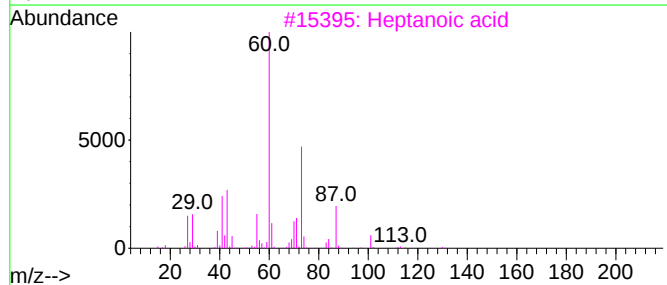
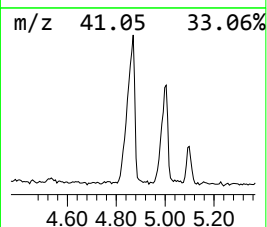
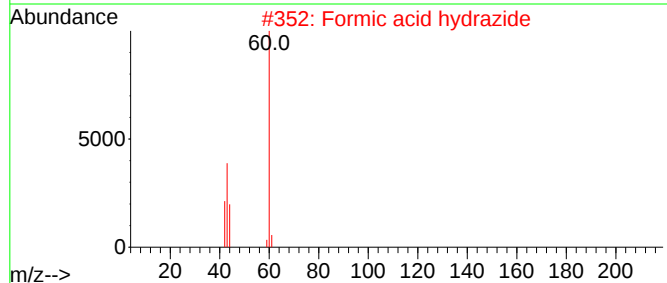
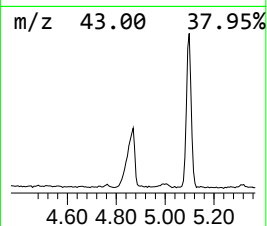
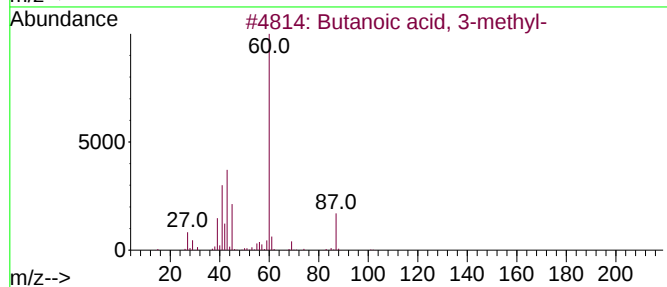
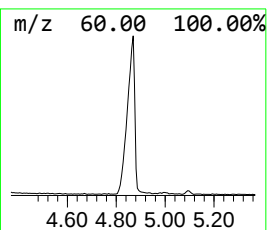
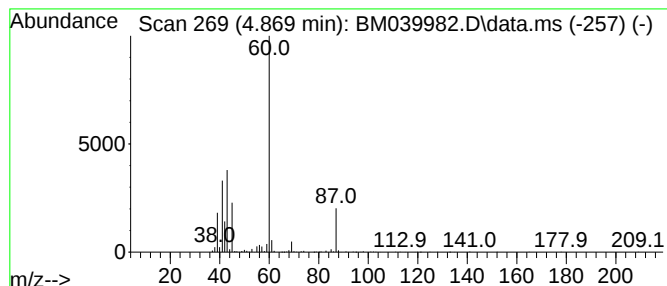
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.869	6.85 ng	679105	1,4-Dichlorobenzene-d4	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2			Formic acid hydrazide	60	CH4N2O	000624-84-0	9
3			Heptanoic acid	130	C7H14O2	000111-14-8	9
4			1-Hexanamine	101	C6H15N	000111-26-2	9
5			Pentanoic acid	102	C5H10O2	000109-52-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

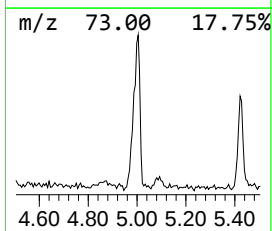
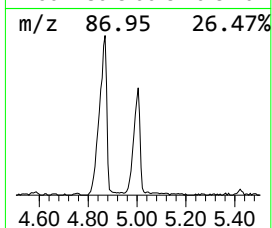
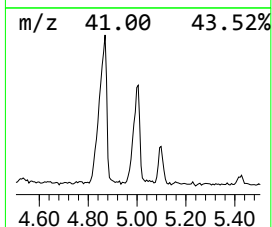
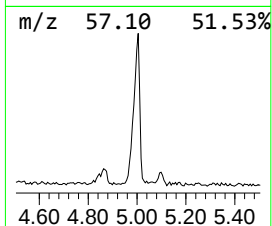
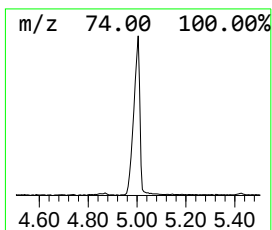
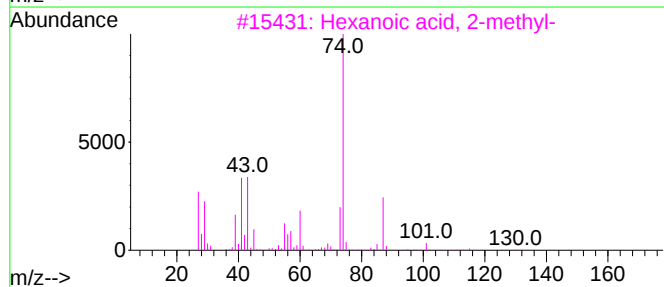
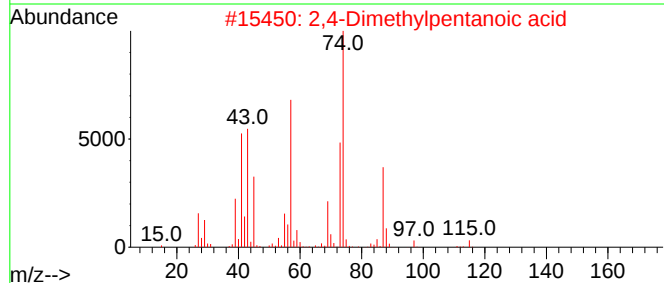
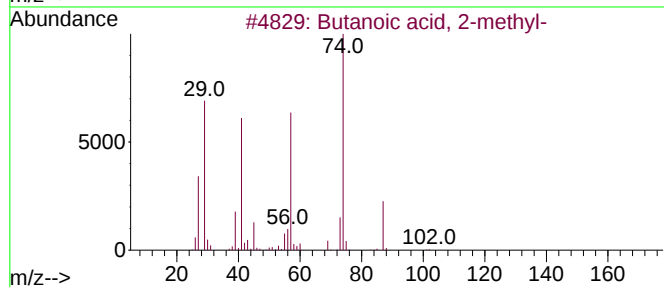
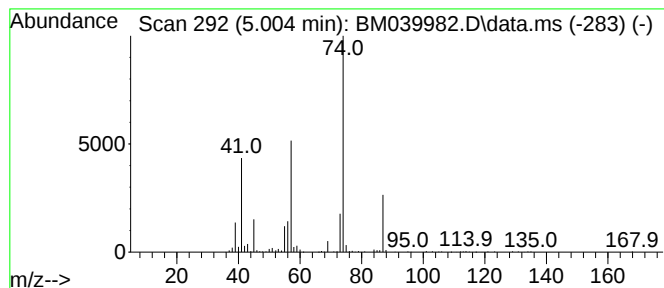
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	3.37 ng	334192	1,4-Dichlorobenzene-d4	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2			2,4-Dimethylpentanoic acid	130	C7H14O2	005868-33-7	72
3			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	56
4			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	50
5			Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

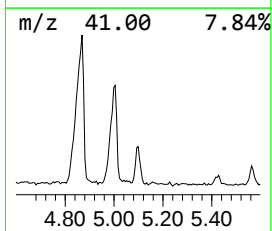
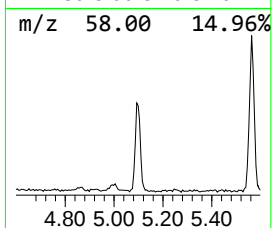
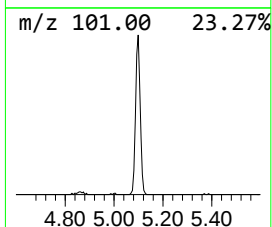
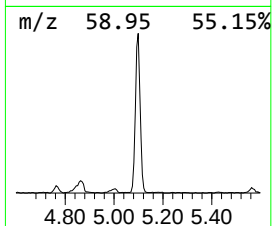
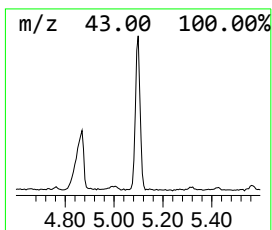
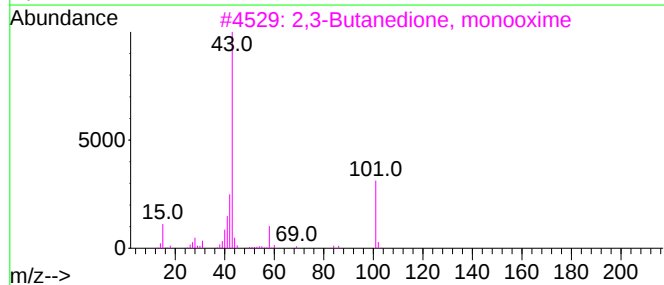
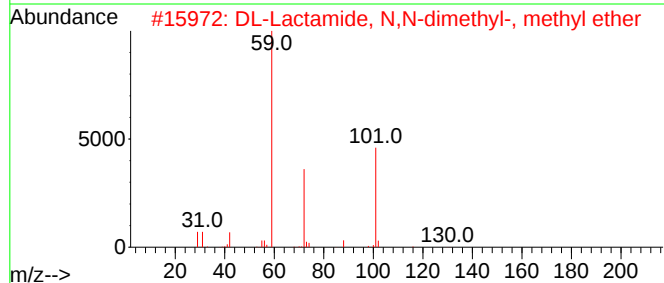
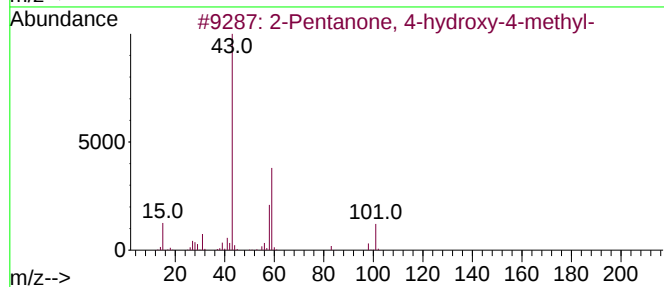
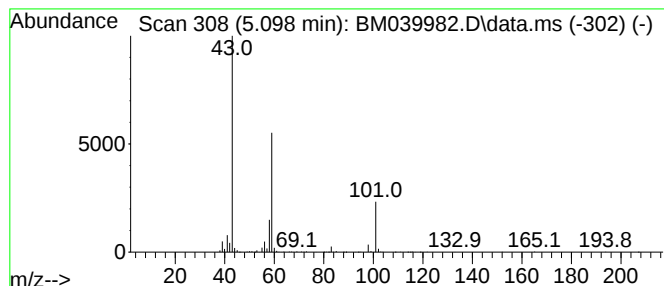
Instrument :
BNA_M
ClientSampleId :
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.098	3.62 ng	358832	1,4-Dichlorobenzene-d4	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

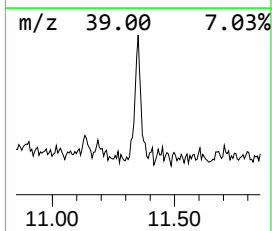
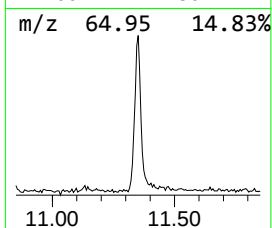
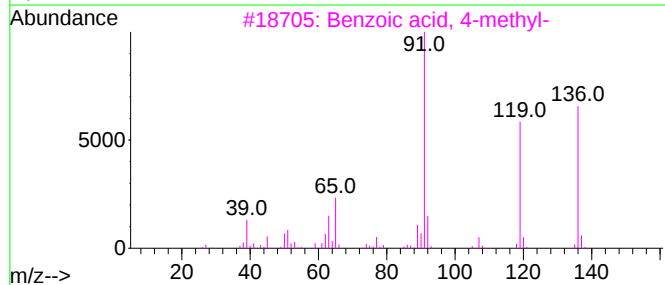
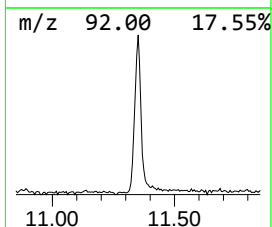
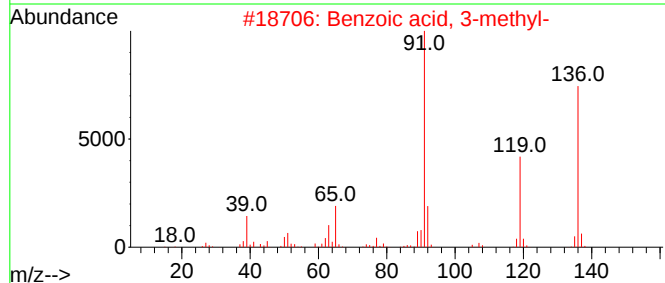
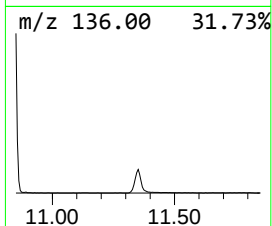
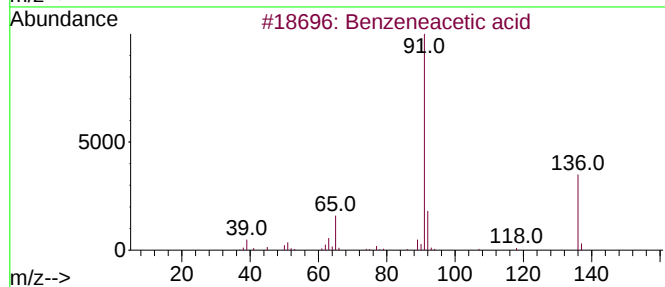
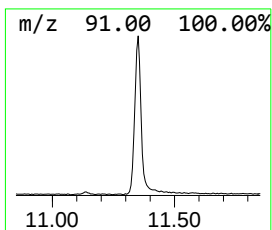
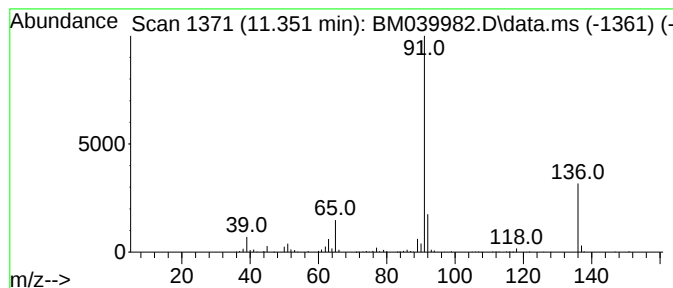
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzeneacetic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.351	2.58 ng	334445	Naphthalene-d8	10.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	72
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59
4			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	53
5			3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

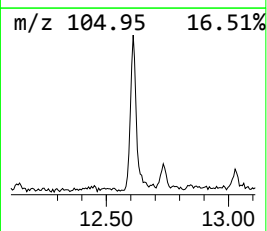
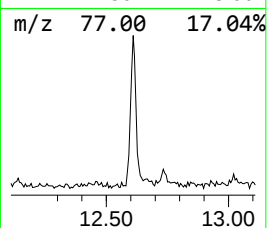
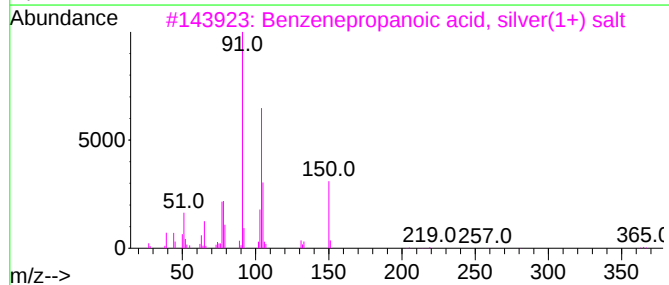
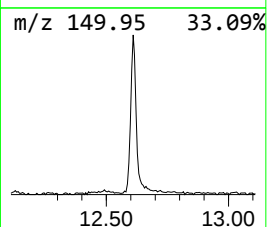
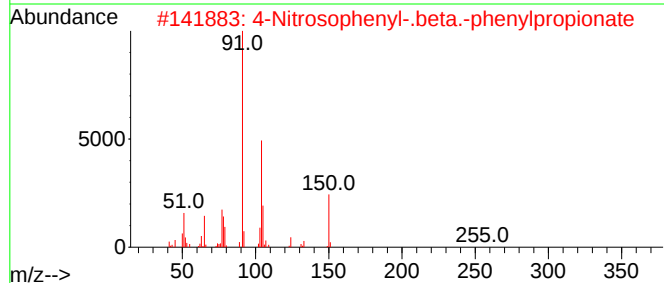
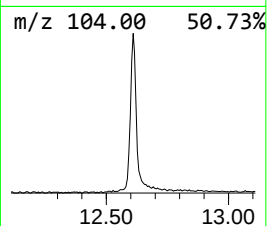
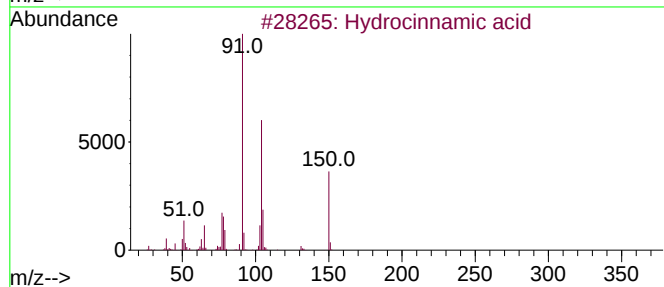
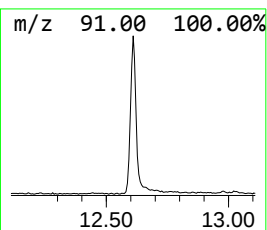
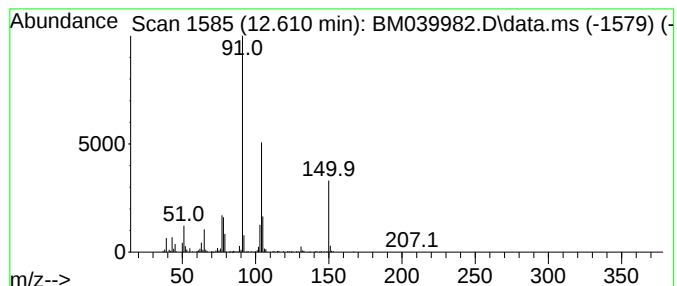
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hydrocinnamic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	3.20 ng	415110	Naphthalene-d8	10.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3			Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	86
4			Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	72
5			Benzenepropanoic acid, octyl ester	262	C17H26O2	037826-57-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

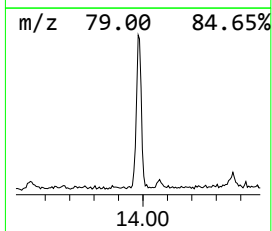
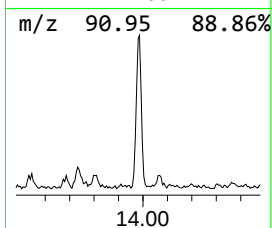
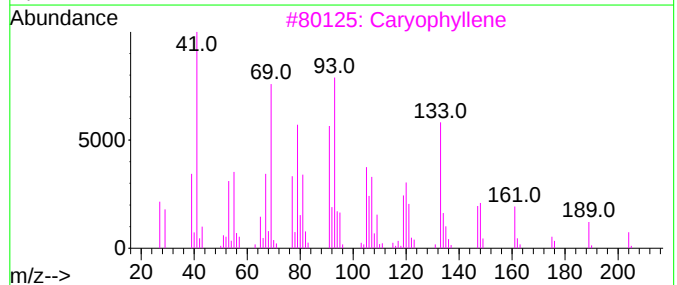
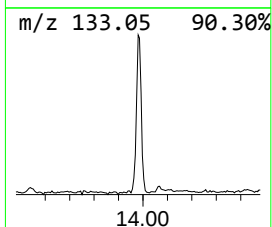
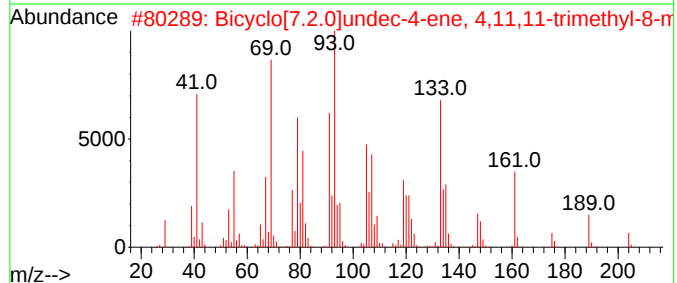
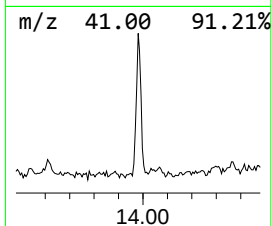
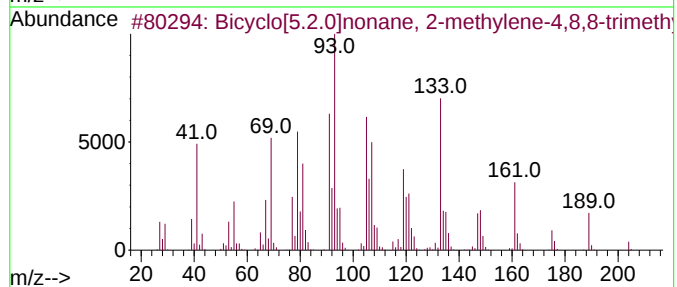
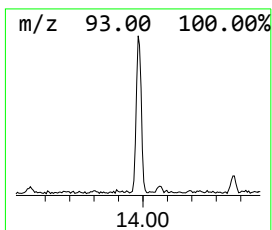
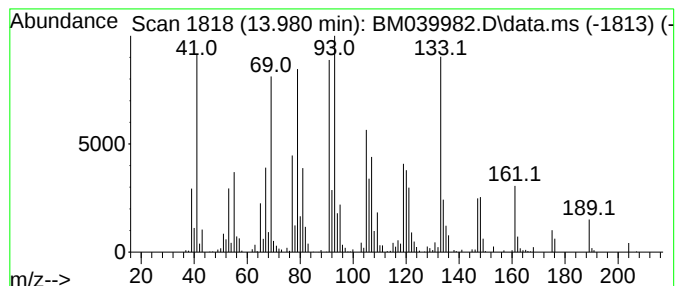
Instrument :
BNA_M
ClientSampleId :
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bicyclo[5.2.0]nonane, 2-met... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.980	2.60 ng	384480	Acenaphthene-d10	14.651	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	91
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	91
3	Caryophyllene	204	C15H24	000087-44-5	91
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	86
5	1S,2S,5R-1,4,4-Trimethyltricyclo...	204	C15H24	1000140-07-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

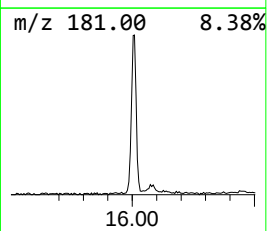
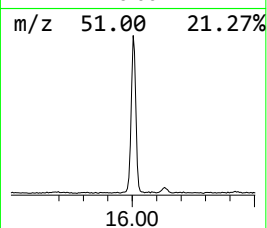
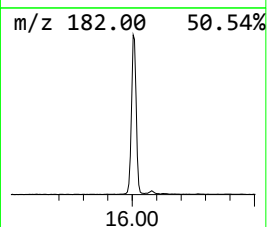
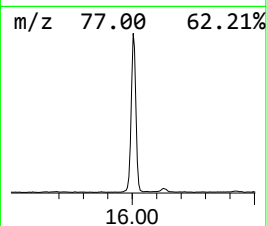
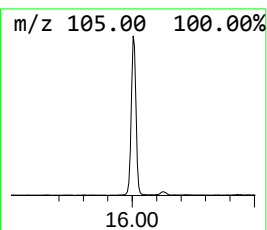
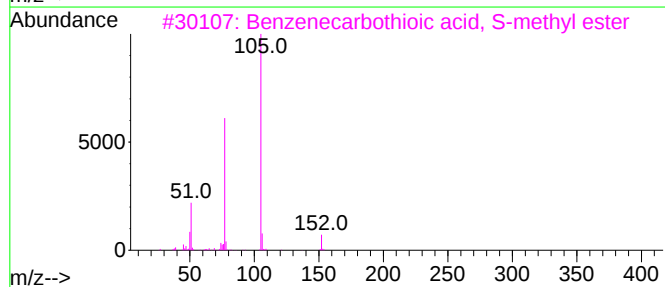
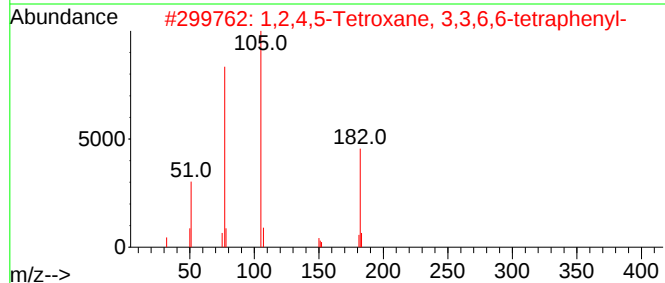
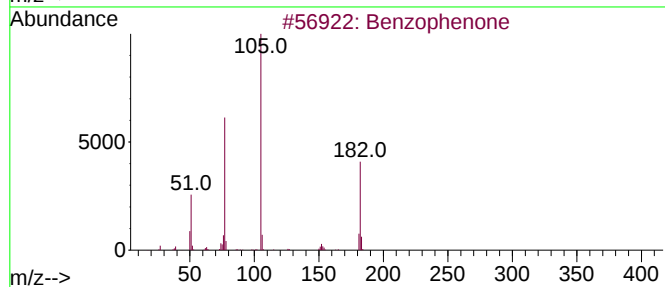
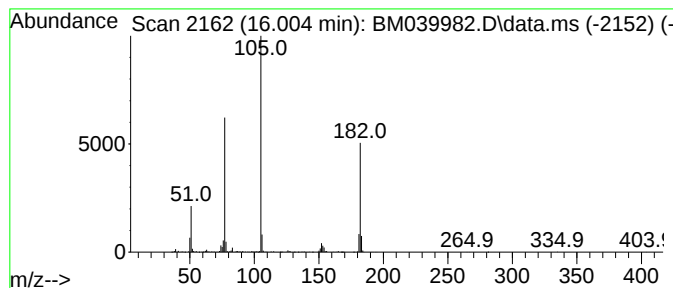
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.003	9.61 ng	1420820	Acenaphthene-d10	14.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

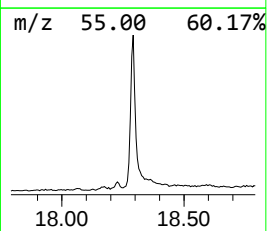
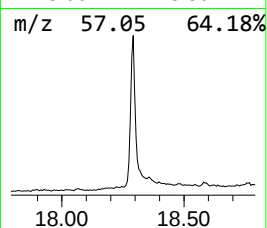
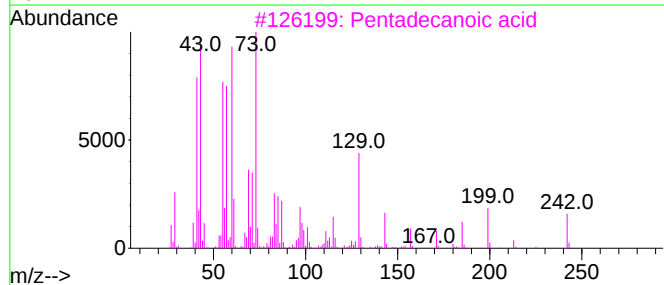
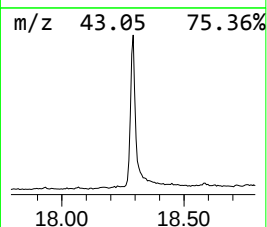
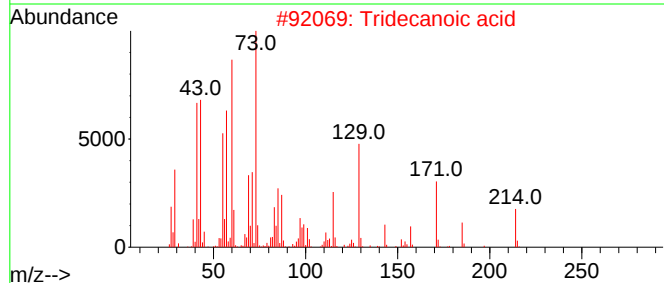
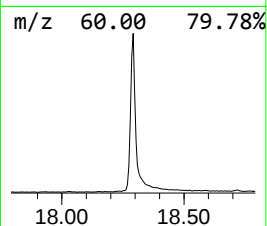
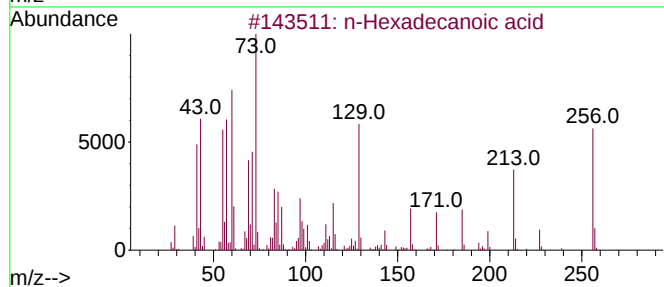
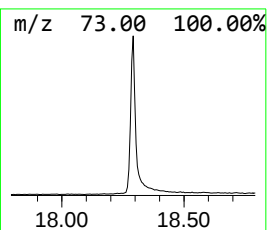
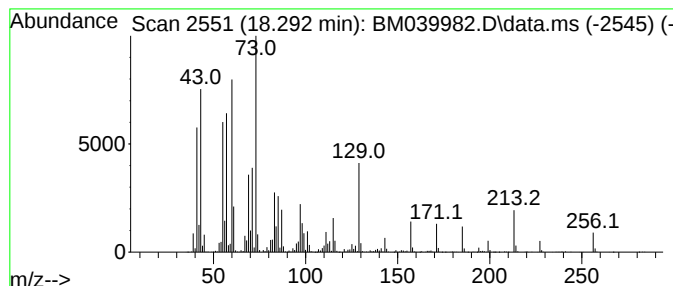
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.292	18.90 ng	3027040	Phenanthrene-d10	17.392

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		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

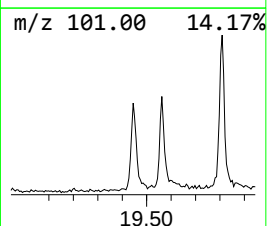
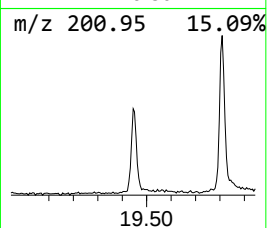
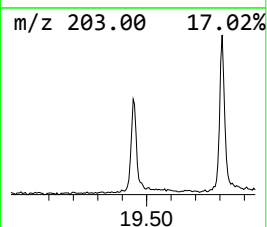
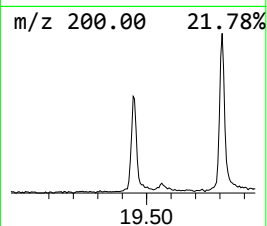
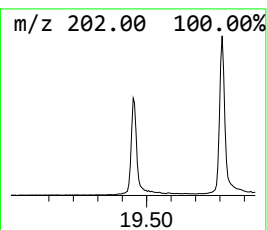
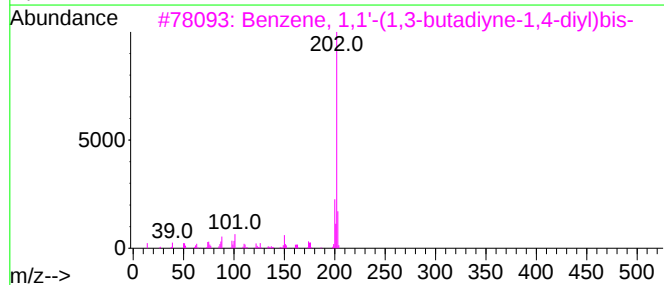
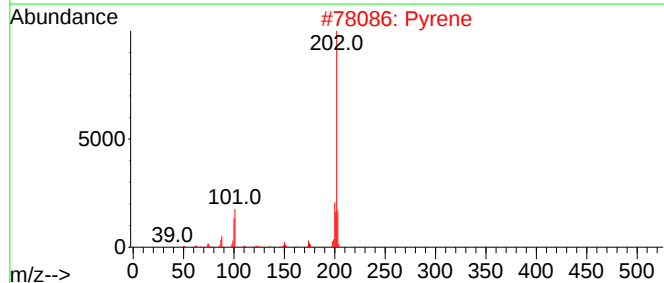
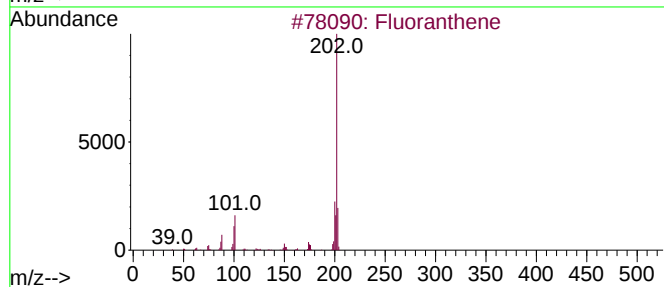
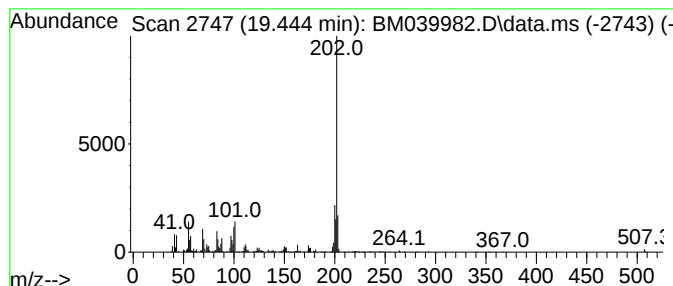
Instrument :
BNA_M
ClientSampleId :
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.445	3.54 ng	566561	Phenanthrene-d10	17.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	98
2	Pyrene	202	C16H10	000129-00-0	96
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	70
4	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	60
5	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

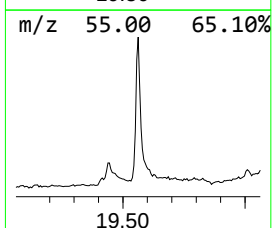
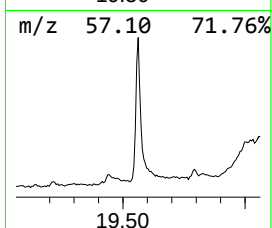
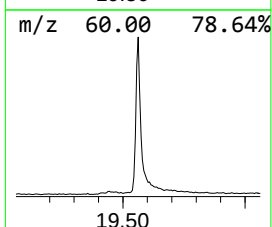
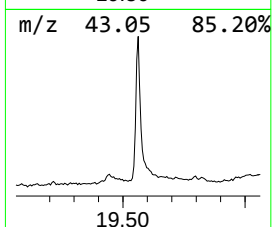
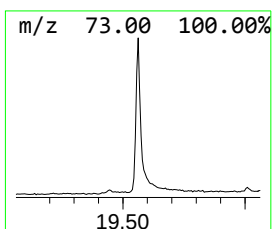
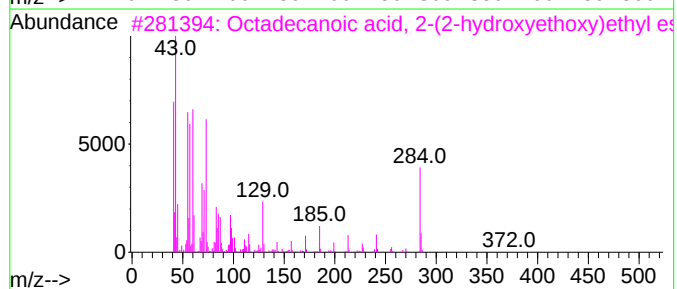
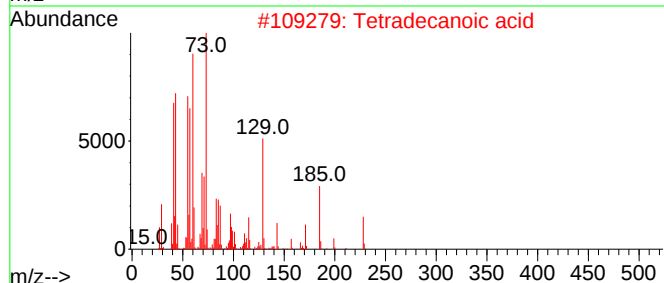
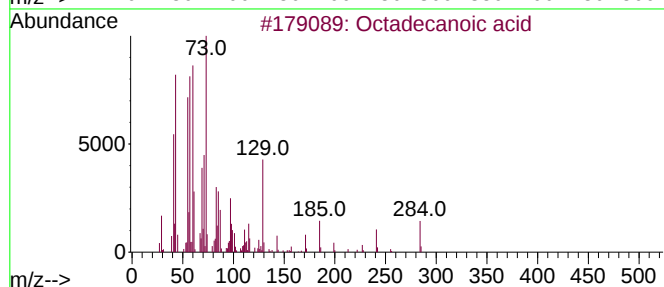
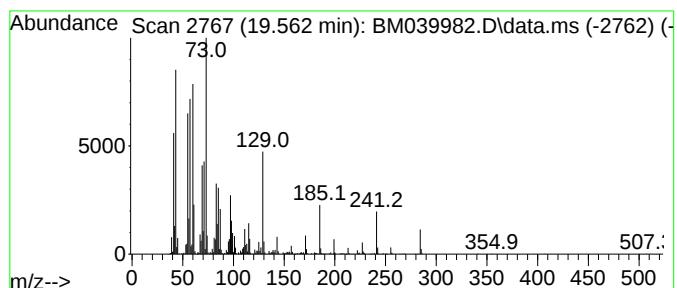
Instrument :
BNA_M
ClientSampleId :
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.562	9.76 ng	2322420	Chrysene-d12	21.574	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

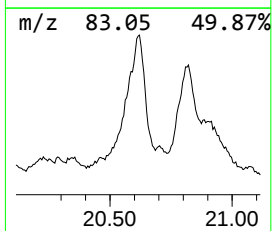
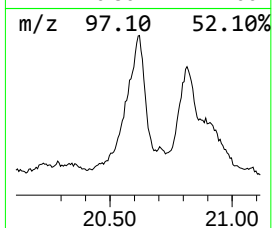
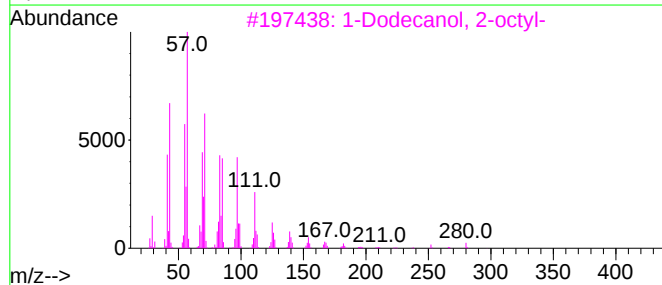
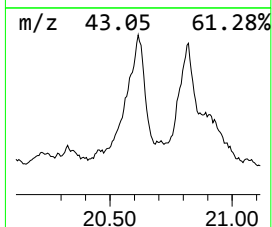
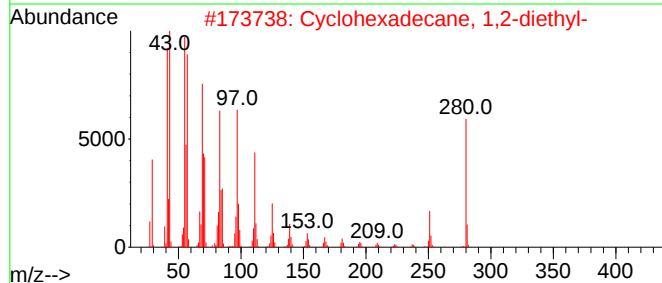
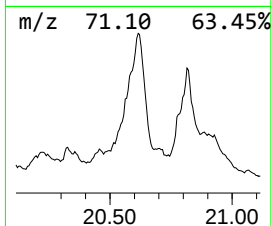
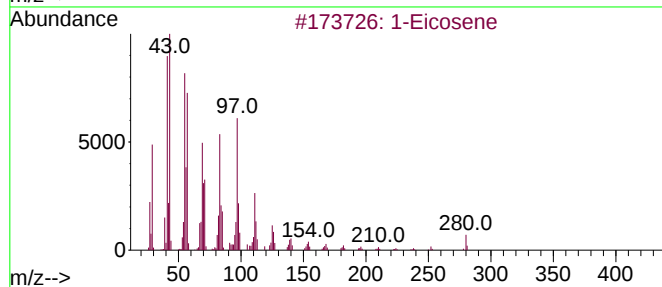
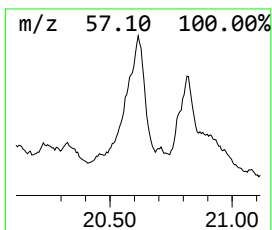
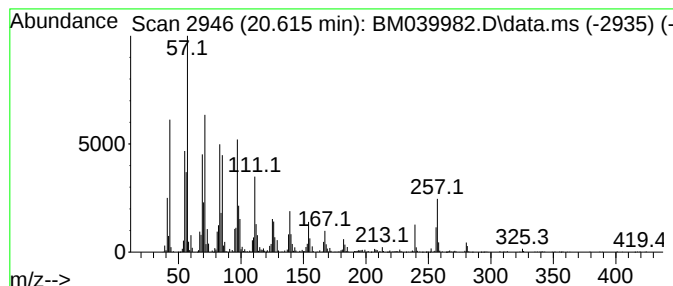
Instrument :
BNA_M
ClientSampleId :
TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Eicosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.615	22.02 ng	5241670	Chrysene-d12	21.574
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1	1-Eicosene		280 C20H40	003452-07-1 91
2	Cyclohexadecane, 1,2-diethyl-		280 C20H40	1000155-85-3 90
3	1-Dodecanol, 2-octyl-		298 C20H42O	005333-42-6 81
4	1-Decanol, 2-hexyl-		242 C16H34O	002425-77-6 74
5	Oxalic acid, isobutyl pentadecyl...		356 C21H40O4	1000309-38-0 74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

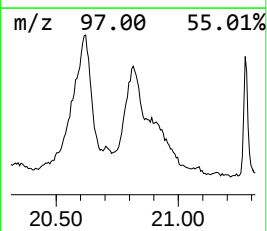
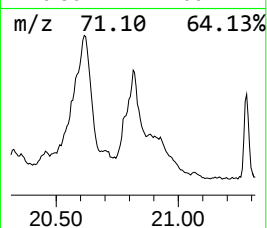
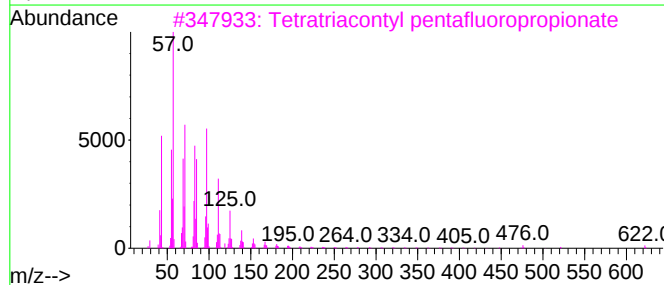
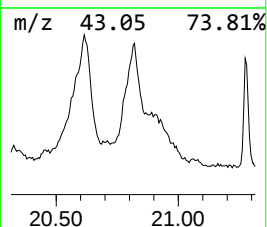
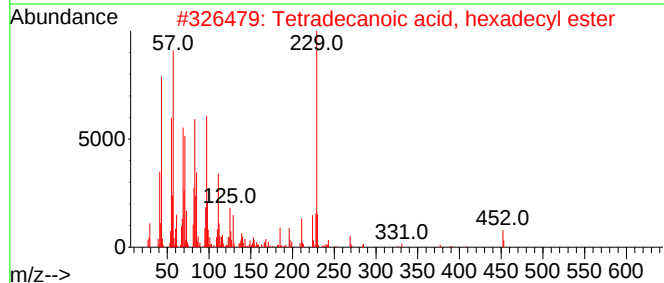
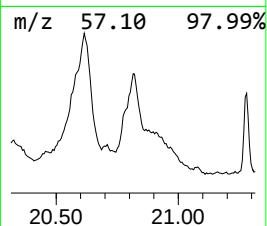
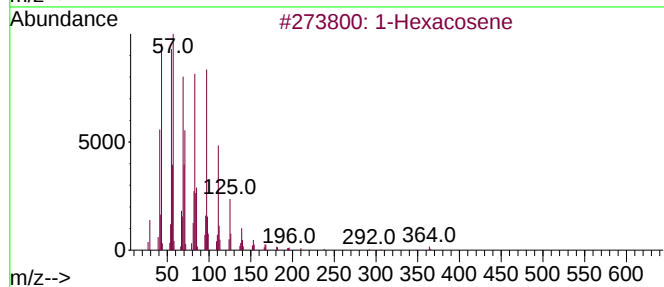
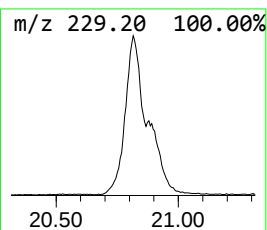
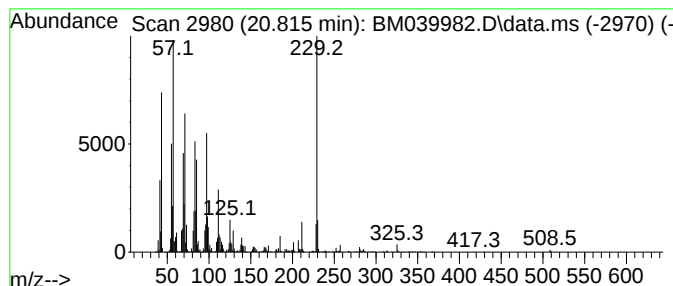
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.815	14.92 ng	3552270	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	87
2	Tetradecanoic acid, hexadecyl ester			452	C30H60O2	002599-01-1	87
3	Tetratriacontyl pentafluoropropi...			641	C37H69F5O2	1000351-81-5	83
4	Dotriacontyl pentafluoropropionate			612	C35H65F5O2	1010351-81-4	83
5	Hexatriacontyl pentafluoropropio...			669	C39H73F5O2	1000351-89-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

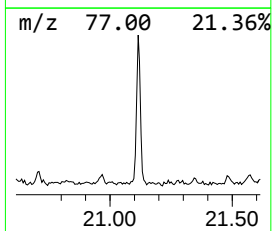
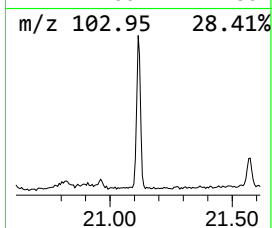
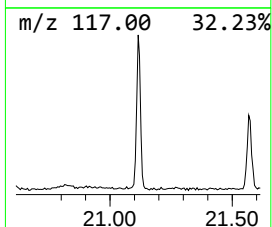
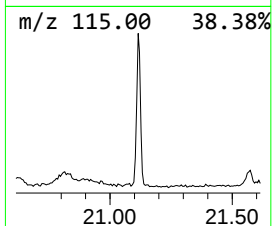
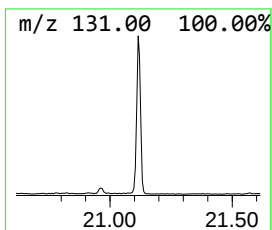
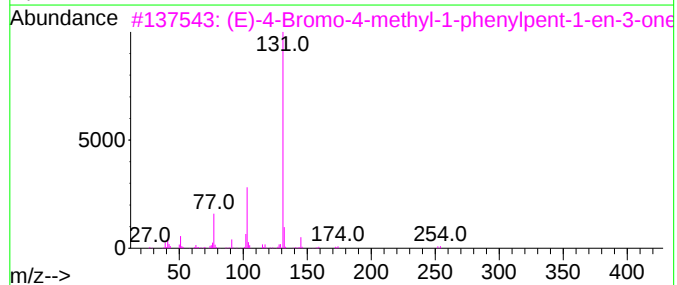
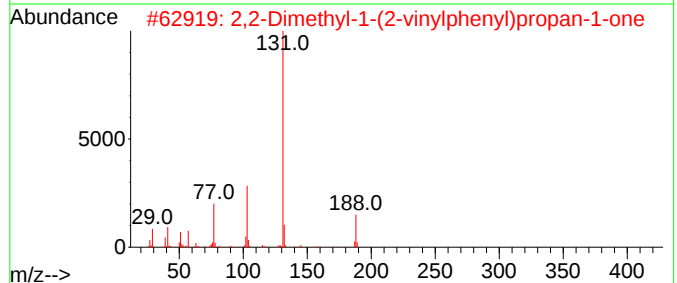
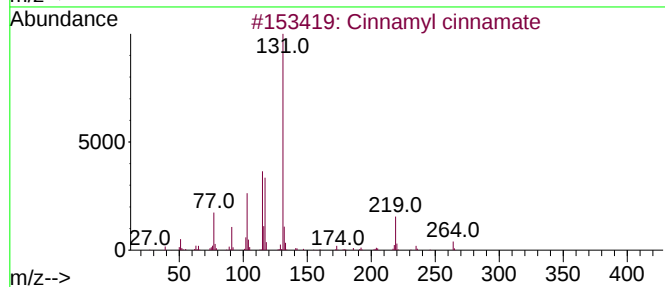
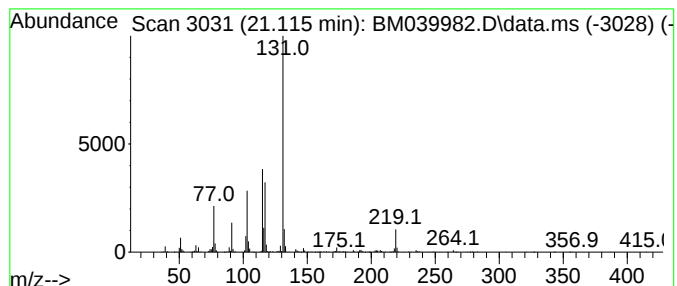
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Cinnamyl cinnamate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.115	2.24 ng	533851	Chrysene-d12	21.574

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2		2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49
3		(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	47
4		(Z)-N-(2-Hydroxyethyl)-3-phenyla...	233	C13H15NO3	1000512-63-0	47
5		(2E)-N-(2-Fluorophenyl)-3-phenyl...	241	C15H12FNO	025893-50-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

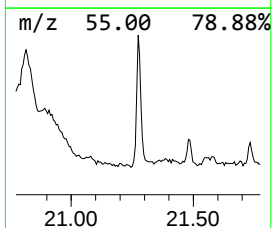
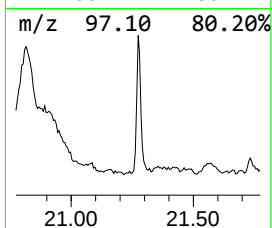
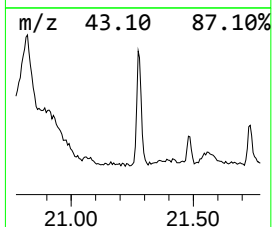
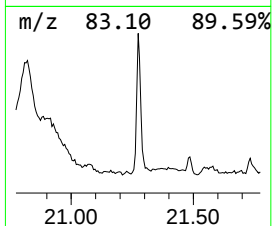
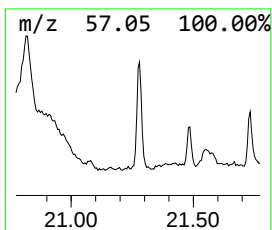
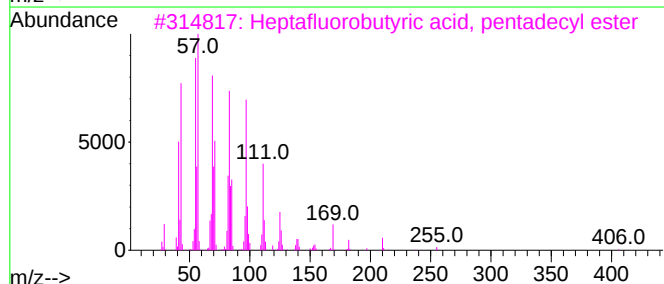
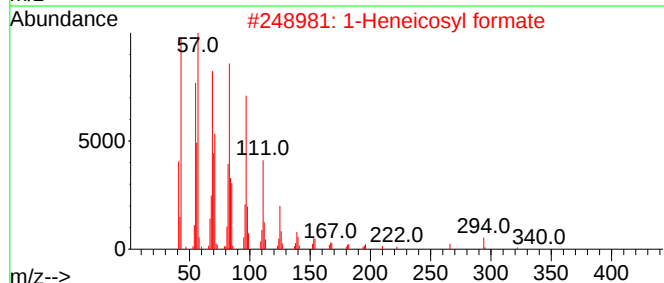
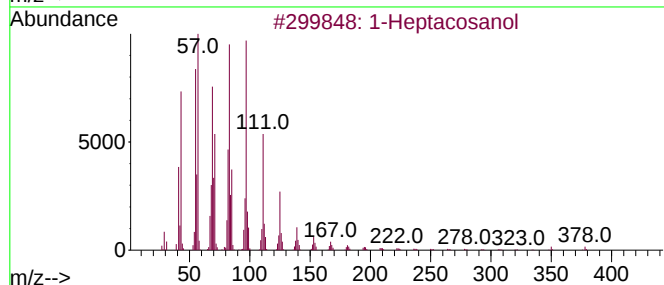
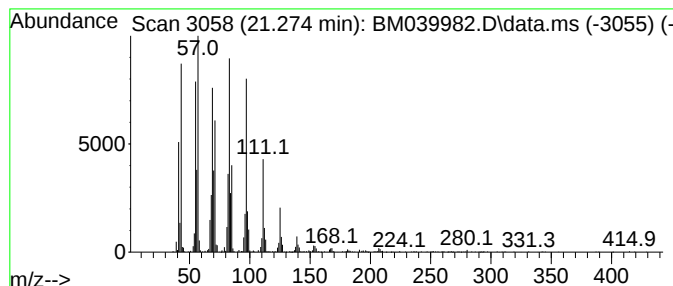
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.274	4.73 ng	1125790	Chrysene-d12	21.574

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	94
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
Data File : BM039982.D
Acq On : 24 May 2023 13:56
Operator : CG/JU
Sample : 02868-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP17

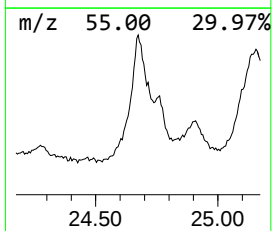
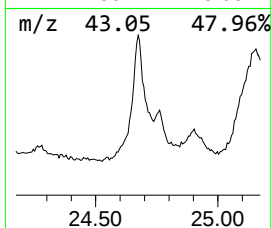
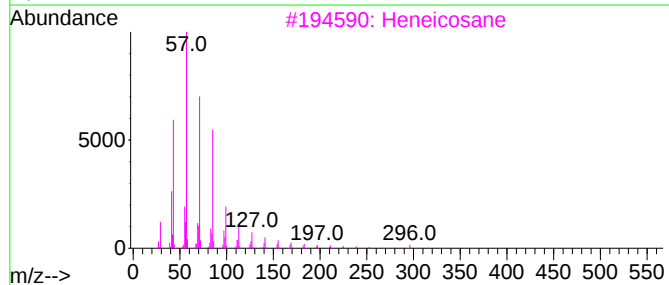
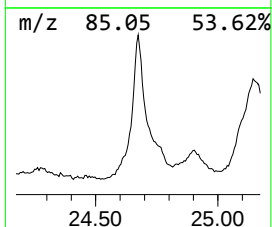
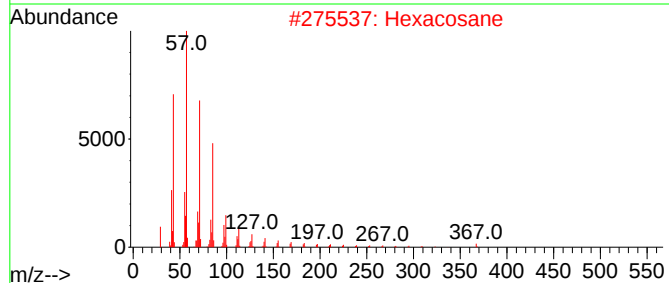
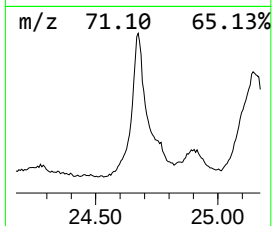
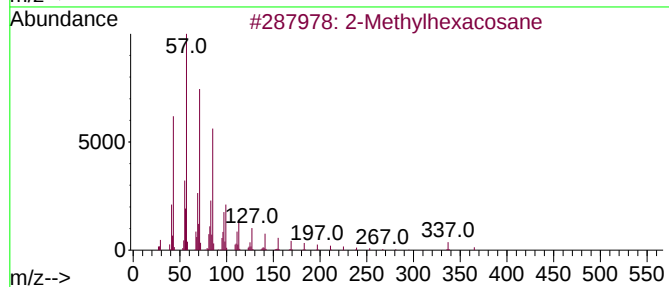
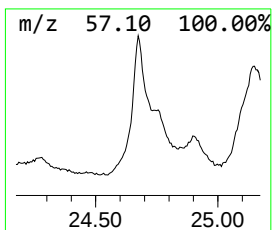
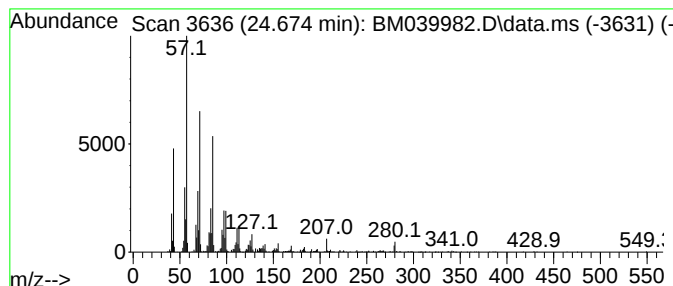
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2-Methylhexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.674	8.31 ng	1629800	Perylene-d12	24.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylhexacosane	380	C27H56	001561-02-0	83
2		Hexacosane	366	C26H54	000630-01-3	68
3		Heneicosane	296	C21H44	000629-94-7	62
4		Octacosane	394	C28H58	000630-02-4	58
5		Heptadecane	240	C17H36	000629-78-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052423\
 Data File : BM039982.D
 Acq On : 24 May 2023 13:56
 Operator : CG/JU
 Sample : 02868-21
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP17

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052323.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
Propanoic acid,...	3.722	8.8	ng	871646	1	8.016	1981400	20.0
Butanoic acid	4.216	87.8	ng	8698100	1	8.016	1981400	20.0
Butanoic acid, ...	4.869	6.8	ng	679105	1	8.016	1981400	20.0
Butanoic acid, ...	5.004	3.4	ng	334192	1	8.016	1981400	20.0
2-Pentanone, 4-...	5.098	3.6	ng	358832	1	8.016	1981400	20.0
Benzeneacetic acid	11.351	2.6	ng	334445	2	10.833	2597570	20.0
Hydrocinnamic acid	12.610	3.2	ng	415110	2	10.833	2597570	20.0
Bicyclo[5.2.0]n...	13.980	2.6	ng	384480	3	14.651	2956830	20.0
Benzophenone	16.003	9.6	ng	1420820	3	14.651	2956830	20.0
n-Hexadecanoic ...	18.292	18.9	ng	3027040	4	17.392	3203900	20.0
Benzene, 1,1'-(...	19.445	3.5	ng	566561	4	17.392	3203900	20.0
Octadecanoic acid	19.562	9.8	ng	2322420	5	21.574	4761130	20.0
1-Eicosene	20.615	22.0	ng	5241670	5	21.574	4761130	20.0
1-Hexacosene	20.815	14.9	ng	3552270	5	21.574	4761130	20.0
Cinnamyl cinnamate	21.115	2.2	ng	533851	5	21.574	4761130	20.0
1-Heptacosanol	21.274	4.7	ng	1125790	5	21.574	4761130	20.0
2-Methylhexacosane	24.674	8.3	ng	1629800	6	24.021	3922860	20.0