

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
 Data File : BM047259.D
 Acq On : 19 Aug 2024 19:29
 Operator : RC/JU
 Sample : P3643-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 917-J-SD-0.5-1-081524

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.569	281	286	293	rVB	93986	138760	3.57%	0.377%
2	5.016	356	362	376	rBV	1865428	2708819	69.65%	7.367%
3	6.575	620	627	639	rBV	1774933	2818434	72.47%	7.665%
4	6.681	639	645	653	rVB	64476	110133	2.83%	0.300%
5	6.998	694	699	706	rBV2	19103	41325	1.06%	0.112%
6	7.363	753	761	771	rBV	847679	1289734	33.16%	3.508%
7	8.510	948	956	966	rBV	1036339	1694955	43.58%	4.610%
8	9.092	1050	1055	1060	rBV	49401	78997	2.03%	0.215%
9	10.116	1221	1229	1237	rBV	1061437	1716280	44.13%	4.668%
10	10.880	1351	1359	1370	rBV	96507	195736	5.03%	0.532%
11	12.627	1649	1656	1669	rBV	1953320	2846148	73.19%	7.741%
12	13.898	1866	1872	1886	rBV5	47296	147273	3.79%	0.401%
13	14.021	1887	1893	1903	rVV	1664871	2375052	61.07%	6.460%
14	14.257	1928	1933	1934	rBV3	57972	71109	1.83%	0.193%
15	14.274	1934	1936	1945	rVB3	71880	100333	2.58%	0.273%
16	15.533	2143	2150	2163	rBV	2371015	3484376	89.60%	9.477%
17	16.786	2357	2363	2368	rBV	2158721	2974914	76.50%	8.091%
18	16.827	2368	2370	2374	rVV	109448	142349	3.66%	0.387%
19	16.868	2374	2377	2381	rVV3	33250	45243	1.16%	0.123%
20	16.921	2382	2386	2392	rVB	34901	52645	1.35%	0.143%
21	16.992	2393	2398	2402	rBV3	20568	40059	1.03%	0.109%
22	17.721	2517	2522	2530	rBV	447853	735773	18.92%	2.001%
23	17.856	2542	2545	2550	rVB2	30601	43007	1.11%	0.117%
24	18.862	2711	2716	2721	rBV	438472	622705	16.01%	1.694%
25	19.027	2739	2744	2755	rBV	208439	427704	11.00%	1.163%
26	19.233	2771	2779	2784	rBV	351201	520309	13.38%	1.415%
27	19.450	2811	2816	2827	rVB	2925339	3573816	91.90%	9.720%
28	19.845	2880	2883	2886	rVB2	44779	49570	1.27%	0.135%
29	20.762	3036	3039	3043	rBV5	128349	156497	4.02%	0.426%
30	21.027	3078	3084	3088	rBV	2811476	3888954	100.00%	10.577%
31	21.062	3088	3090	3099	rVB	268690	359227	9.24%	0.977%
32	23.727	3536	3543	3560	rVB	1405341	3317725	85.31%	9.023%

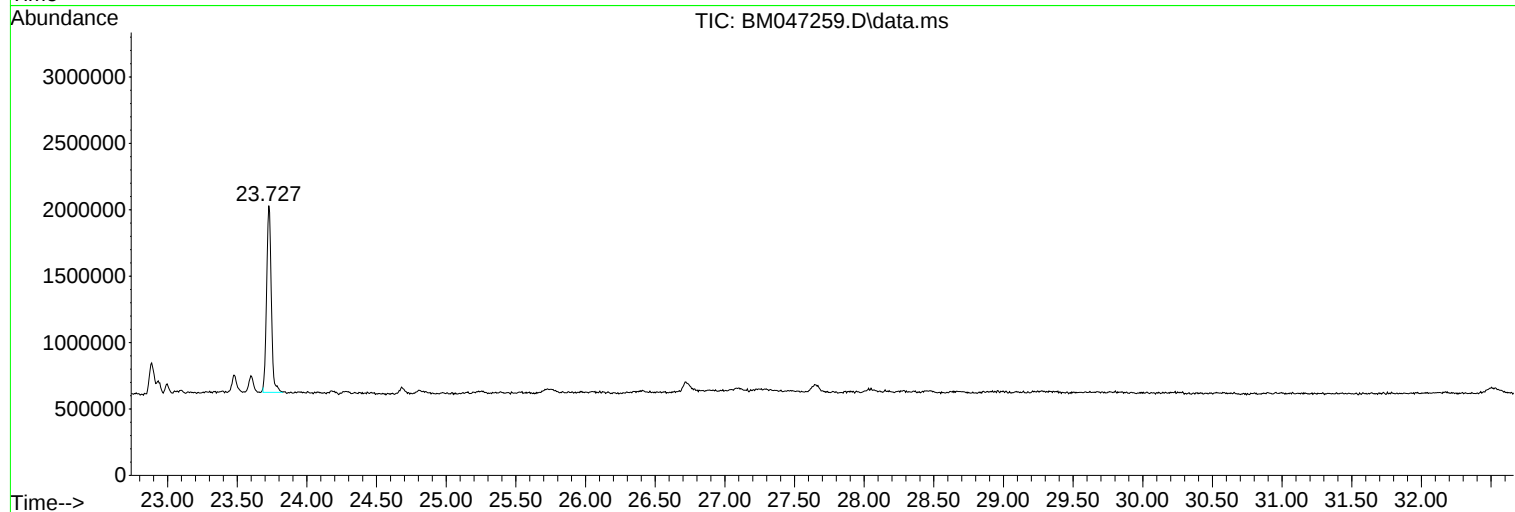
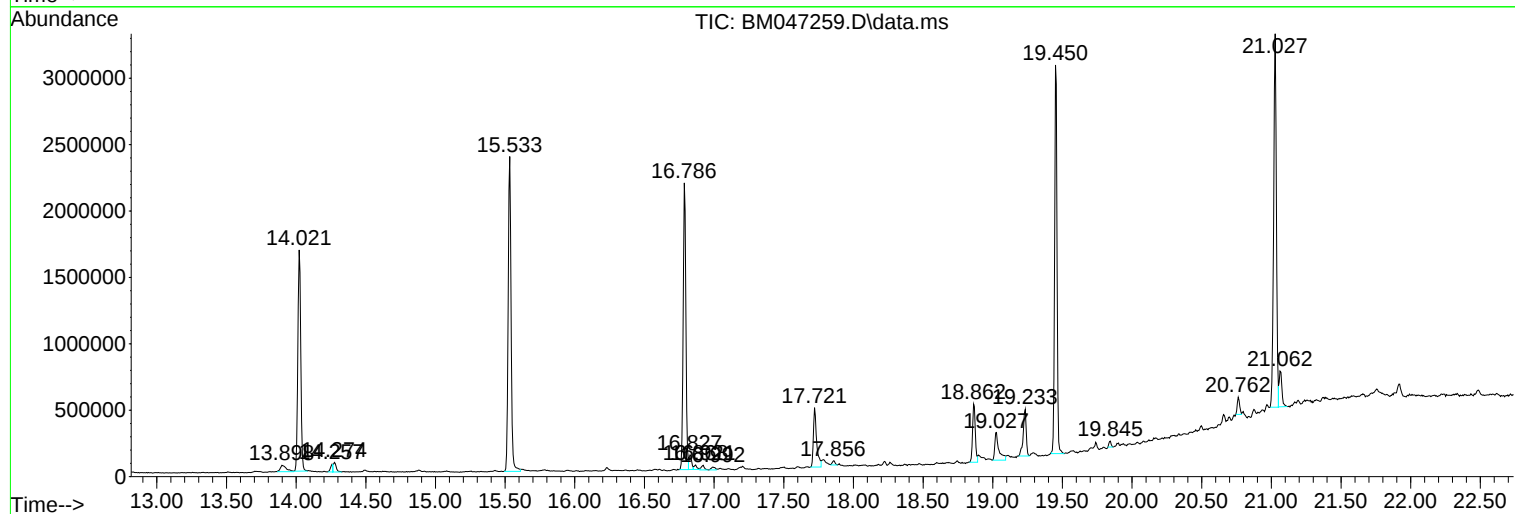
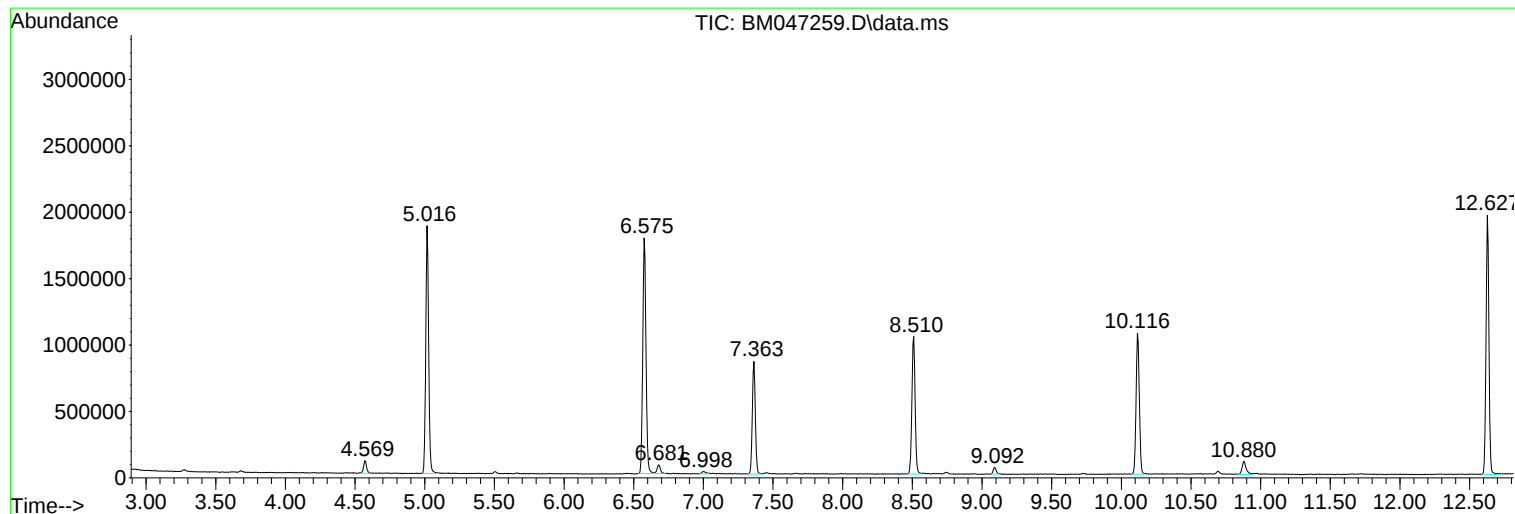
Sum of corrected areas: 36767961

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047259.D
Acq On : 19 Aug 2024 19:29
Operator : RC/JU
Sample : P3643-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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\BM081924\
Data File : BM047259.D
Acq On : 19 Aug 2024 19:29
Operator : RC/JU
Sample : P3643-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0.5-1-081524

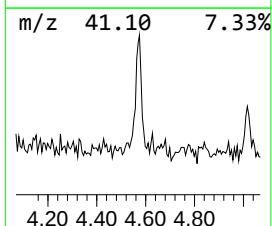
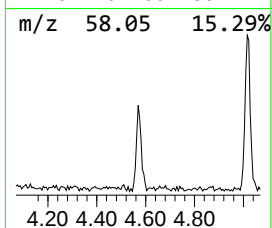
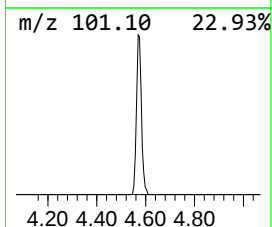
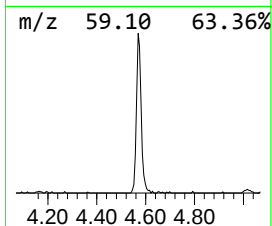
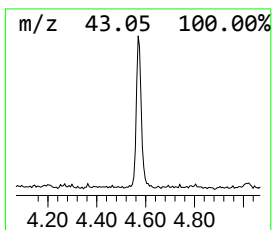
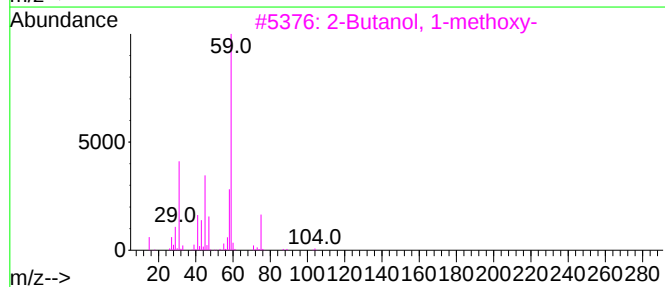
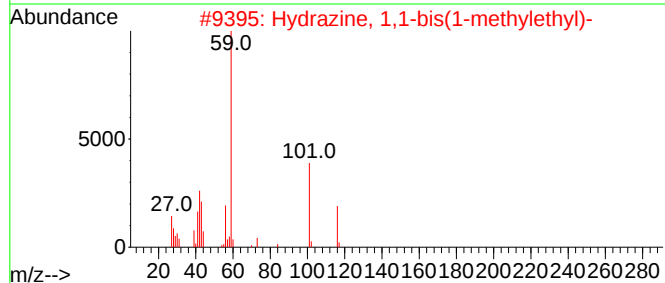
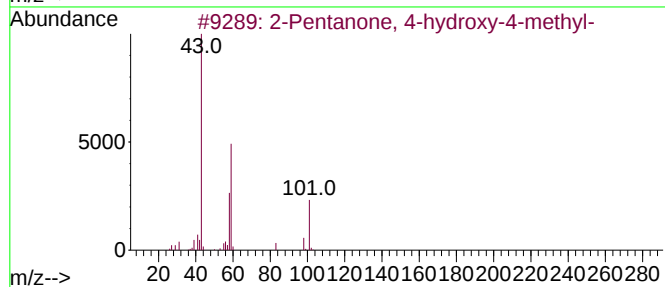
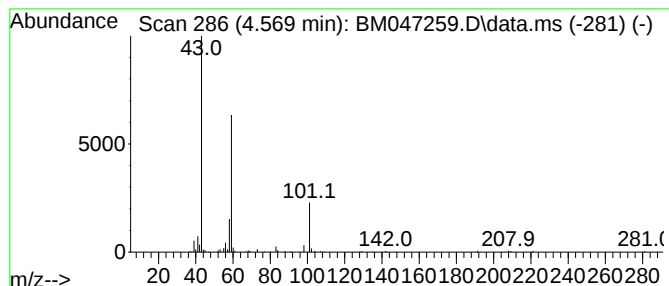
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	2.15 ng	138760	1,4-Dichlorobenzene-d4	7.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33	
3	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	32	
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25	
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047259.D
Acq On : 19 Aug 2024 19:29
Operator : RC/JU
Sample : P3643-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0.5-1-081524

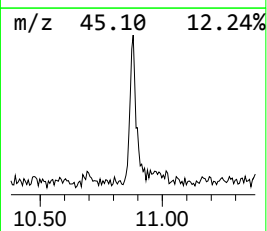
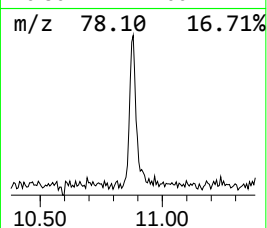
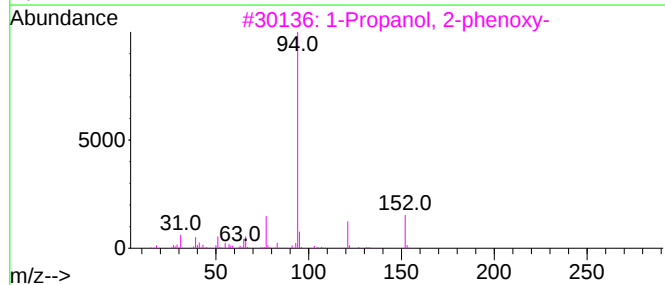
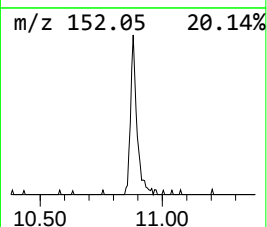
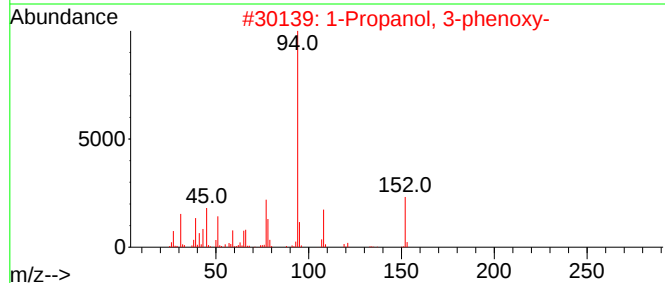
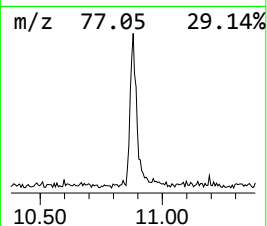
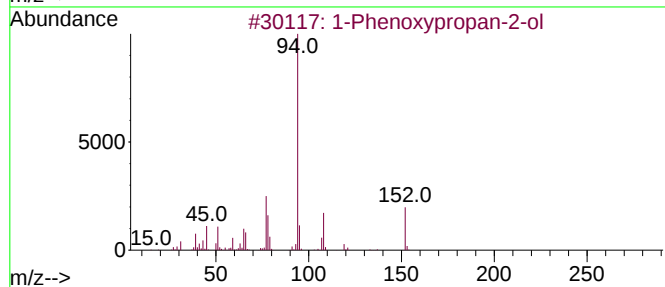
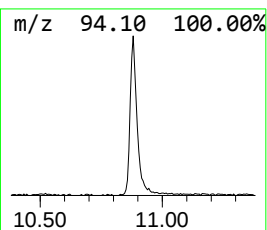
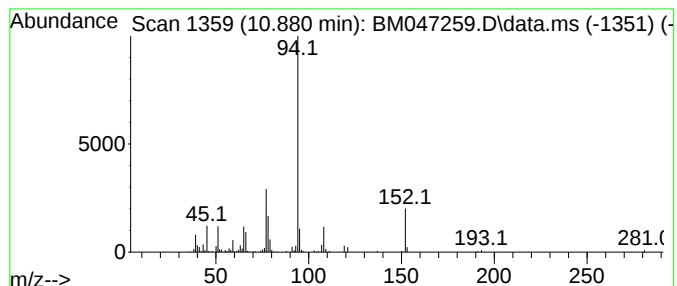
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.880	2.28 ng	195736	Naphthalene-d8	10.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	93
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	72
4			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53
5			Benzene, propoxy-	136	C9H12O	000622-85-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047259.D
Acq On : 19 Aug 2024 19:29
Operator : RC/JU
Sample : P3643-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0.5-1-081524

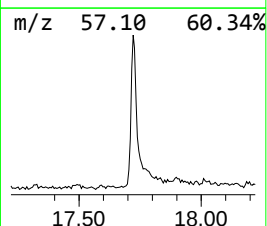
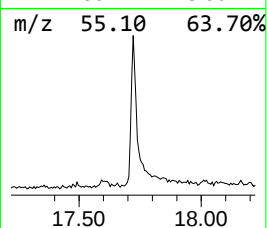
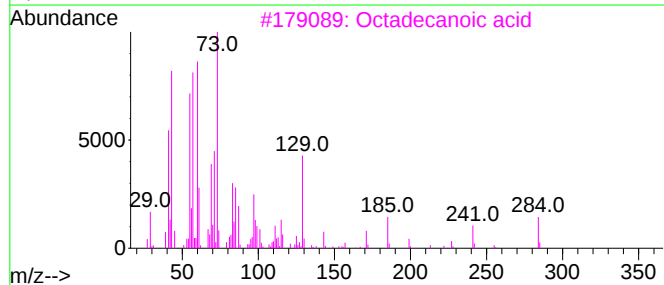
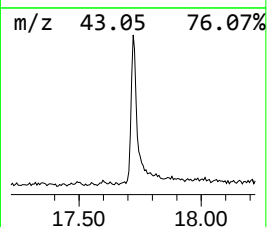
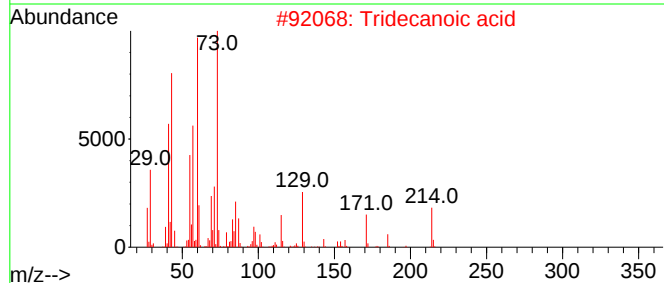
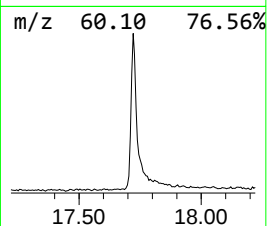
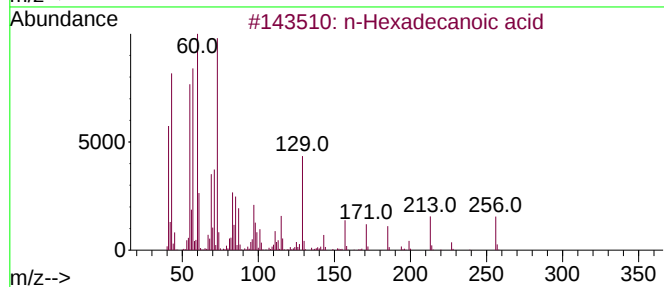
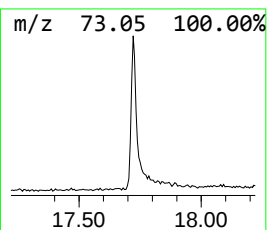
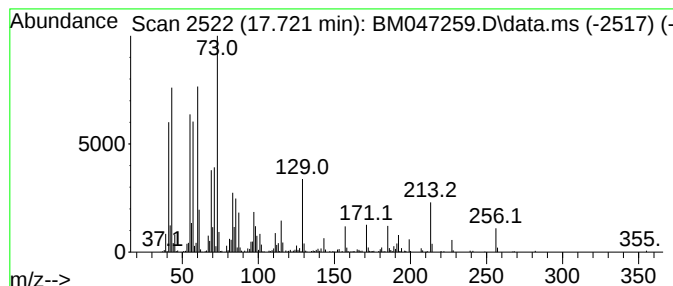
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.721	4.95 ng	735773	Phenanthrene-d10	16.786

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			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047259.D
Acq On : 19 Aug 2024 19:29
Operator : RC/JU
Sample : P3643-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0.5-1-081524

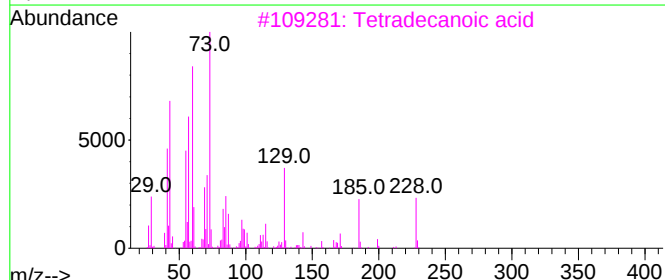
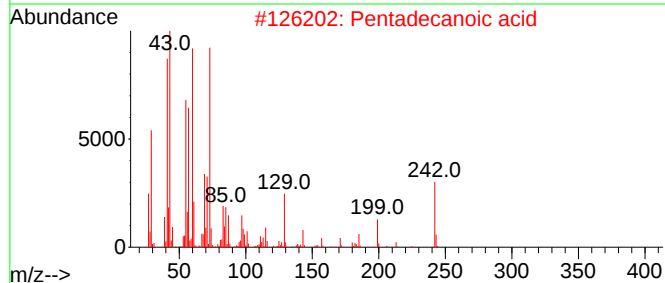
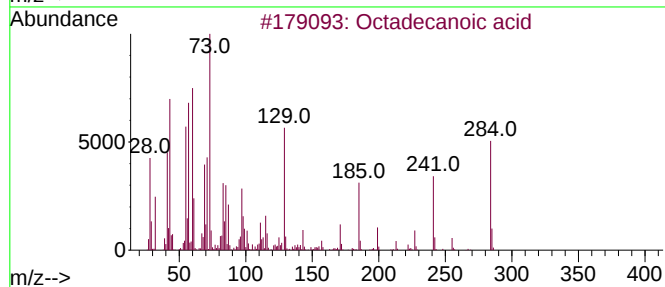
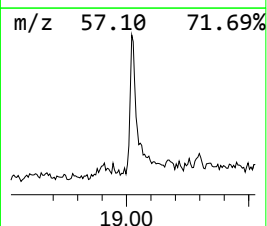
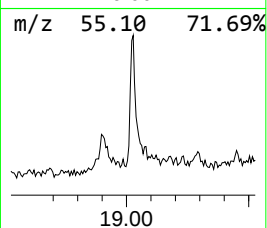
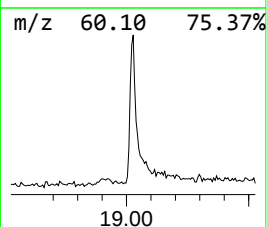
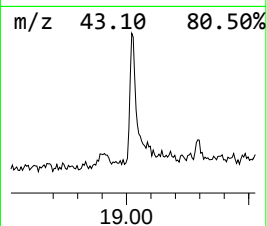
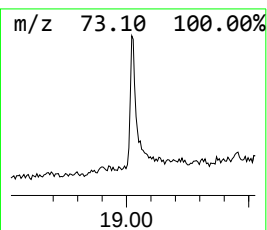
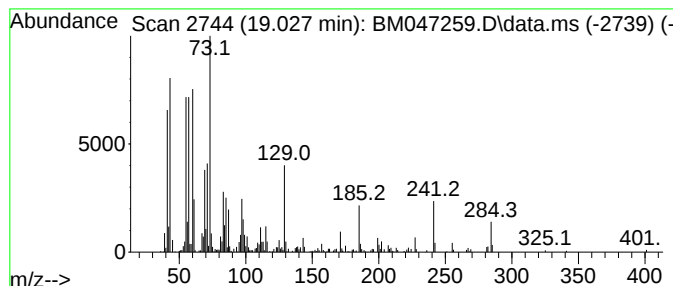
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	2.20 ng	427704	Chrysene-d12	21.027

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
Data File : BM047259.D
Acq On : 19 Aug 2024 19:29
Operator : RC/JU
Sample : P3643-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
917-J-SD-0.5-1-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.569	2.1	ng	138760	1	7.363	1289730	20.0
1-Phenoxypropan...	10.880	2.3	ng	195736	2	10.116	1716280	20.0
n-Hexadecanoic ...	17.721	5.0	ng	735773	4	16.786	2974910	20.0
Octadecanoic acid	19.027	2.2	ng	427704	5	21.027	3888950	20.0