

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
 Data File : BM037480.D
 Acq On : 11 Nov 2022 23:07
 Operator : CG/JU
 Sample : N5530-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-11

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-BM102822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037480.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	46	49	58	rVB	114074	141743	1.22%	0.235%
2	4.299	202	206	212	rBV	135209	173887	1.49%	0.288%
3	4.910	305	310	321	rBV	1243541	1686184	14.48%	2.794%
4	5.375	383	389	403	rBV	4277787	6288103	53.99%	10.418%
5	6.987	656	663	684	rBV	4046368	6461805	55.49%	10.706%
6	7.804	795	802	810	rBV	824854	1297073	11.14%	2.149%
7	8.975	994	1001	1019	rBV	2457000	4061334	34.87%	6.729%
8	10.404	1238	1244	1256	rBV	46793	144073	1.24%	0.239%
9	10.604	1270	1278	1299	rBV	991089	1736894	14.91%	2.878%
10	13.069	1690	1697	1721	rBV	6062833	9154723	78.61%	15.168%
11	14.445	1925	1931	1944	rBV	1374126	2091902	17.96%	3.466%
12	15.939	2175	2185	2203	rBV	4570516	6799177	58.38%	11.265%
13	17.192	2392	2398	2416	rBV	1450049	2254726	19.36%	3.736%
14	18.092	2546	2551	2561	rBV	213892	433907	3.73%	0.719%
15	19.374	2765	2769	2778	rBV	153754	292660	2.51%	0.485%
16	19.821	2840	2845	2857	rBV	9637339	11645807	100.00%	19.295%
17	20.586	2972	2975	2978	rBV	134253	138416	1.19%	0.229%
18	21.092	3057	3061	3069	rBV	307692	487143	4.18%	0.807%
19	21.380	3105	3110	3120	rBV	1853616	2495061	21.42%	4.134%
20	23.721	3502	3508	3520	rVB2	1317991	2570693	22.07%	4.259%

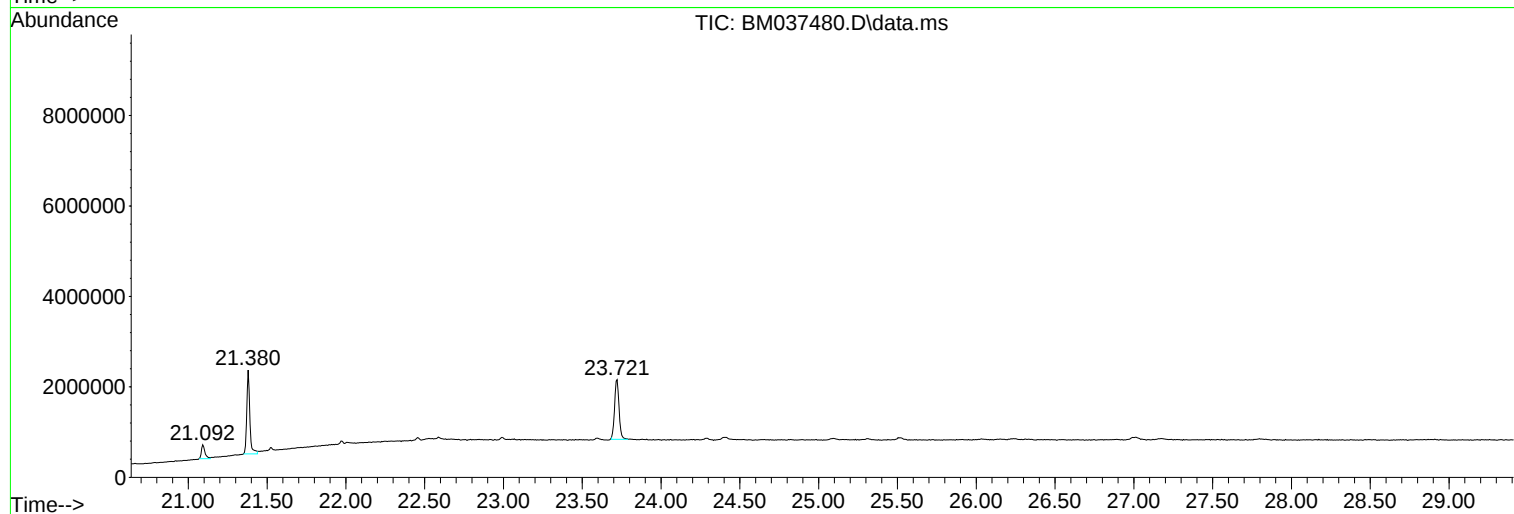
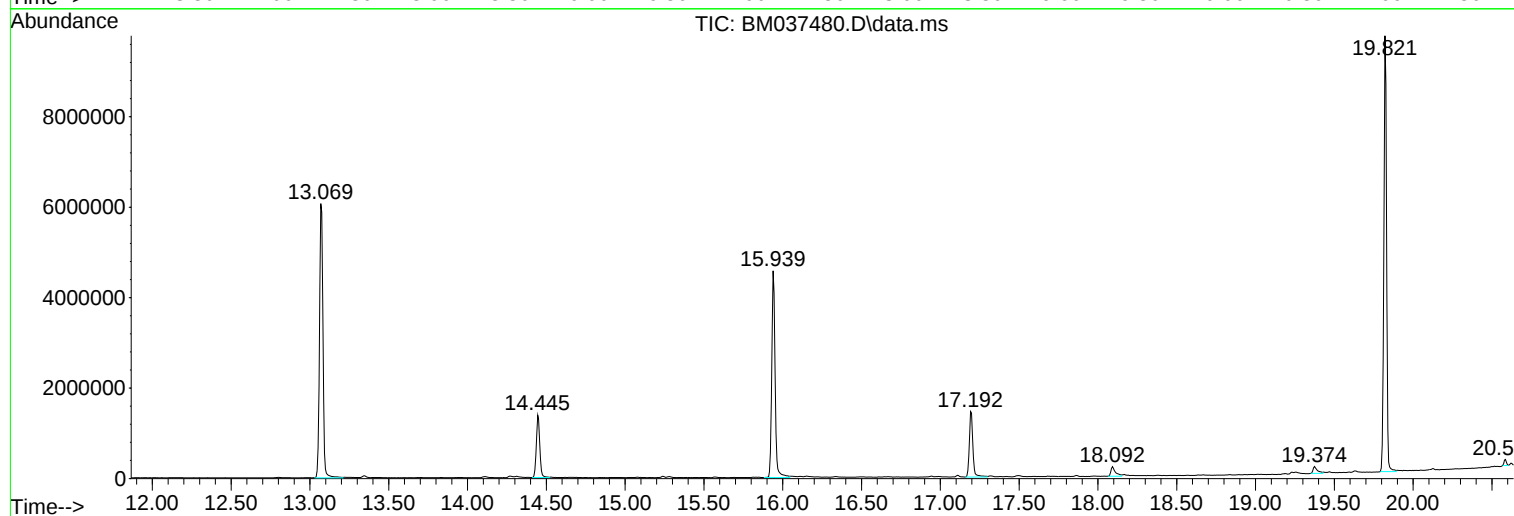
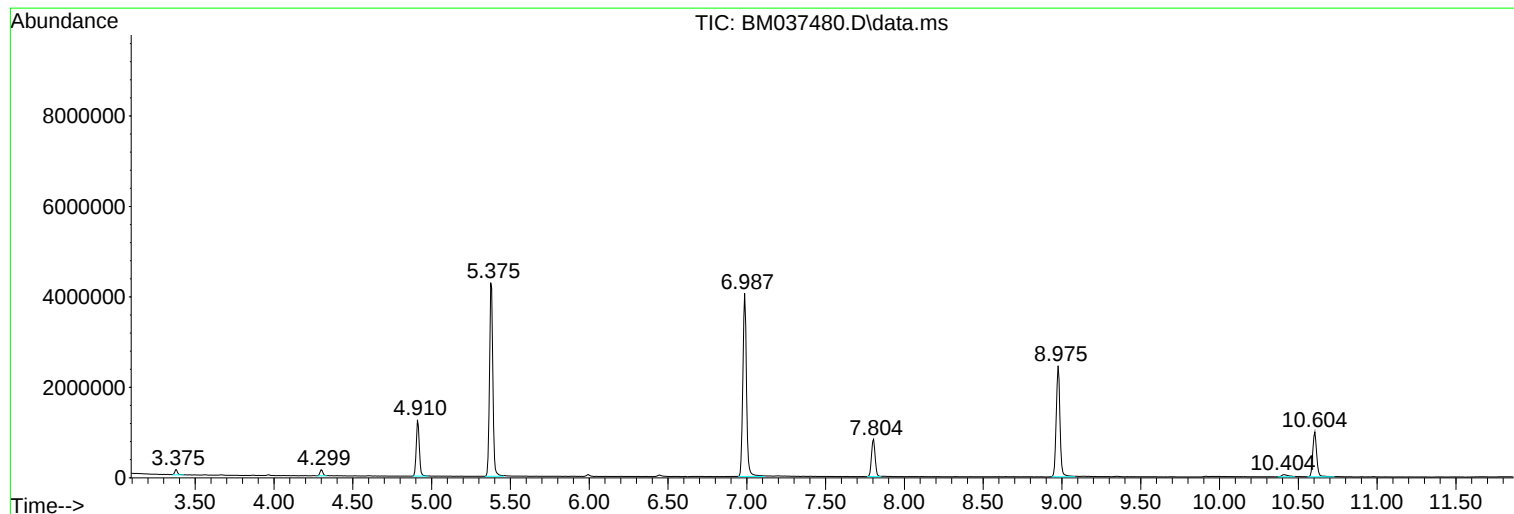
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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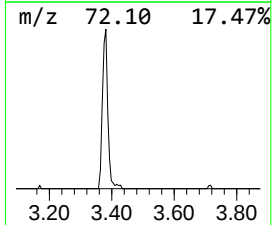
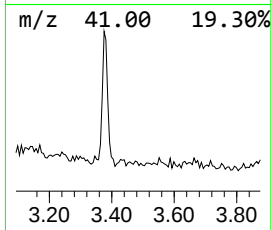
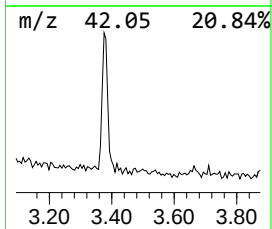
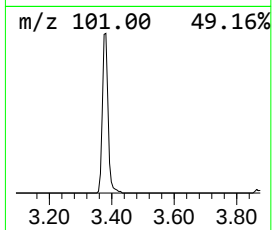
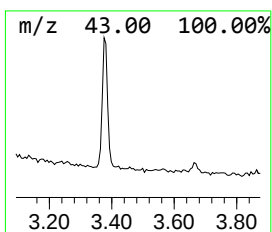
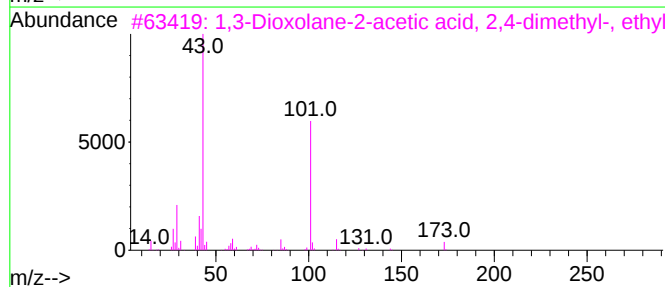
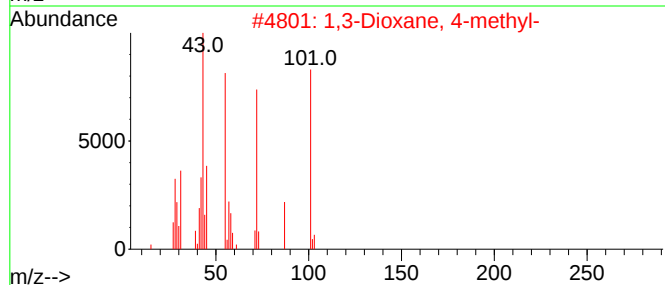
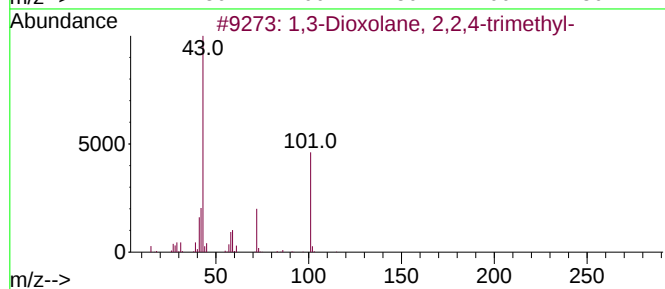
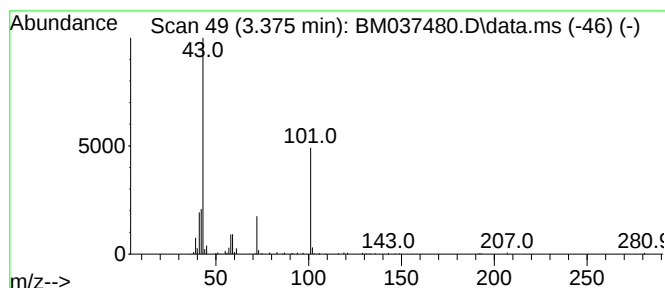
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	2.19 ng	141743	1,4-Dichlorobenzene-d4	7.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
3		1,3-Dioxolane-2-acetic acid, 2,4...	188	C9H16O4	090293-83-7	42
4		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	38
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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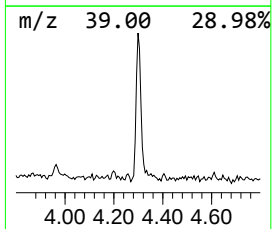
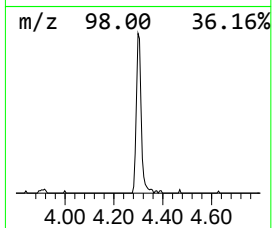
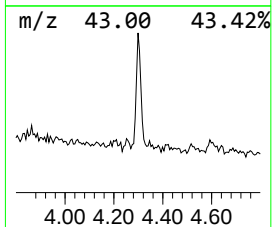
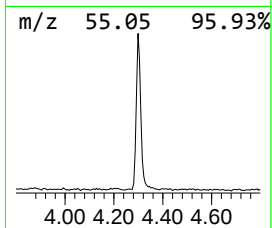
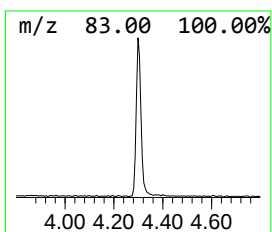
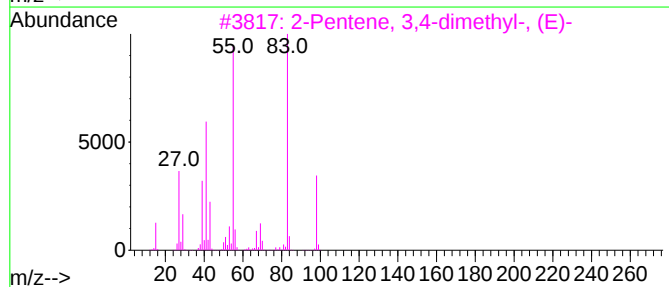
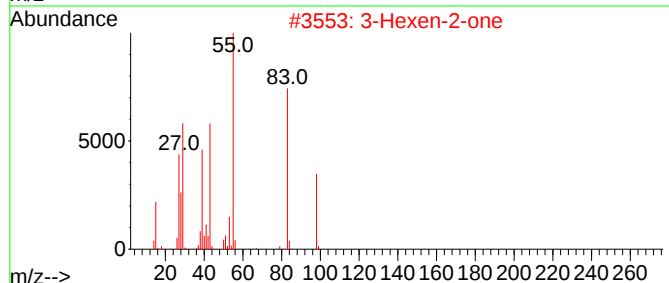
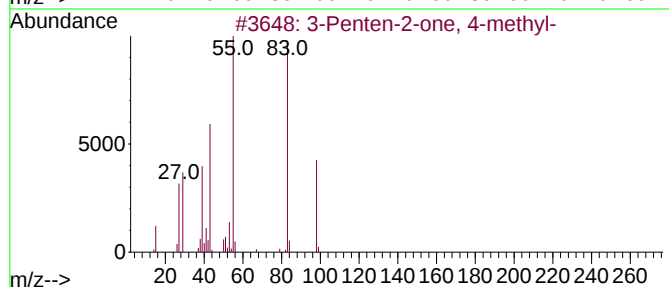
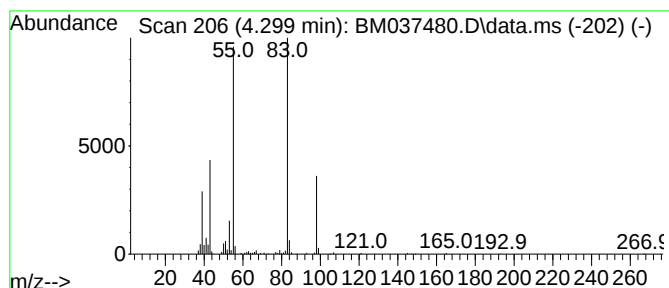
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TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	2.68 ng	173887	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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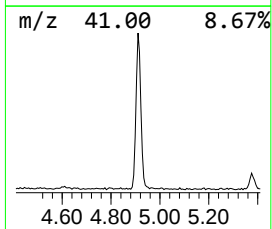
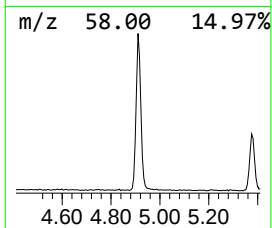
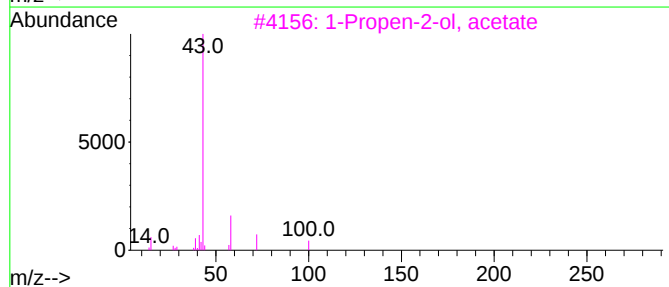
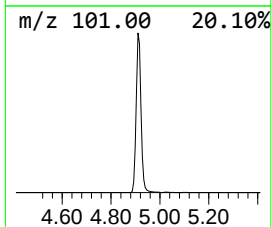
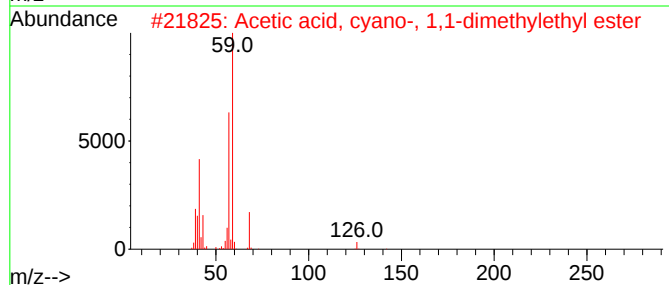
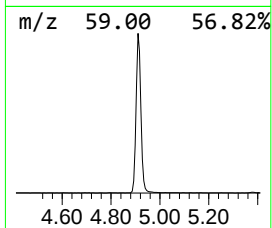
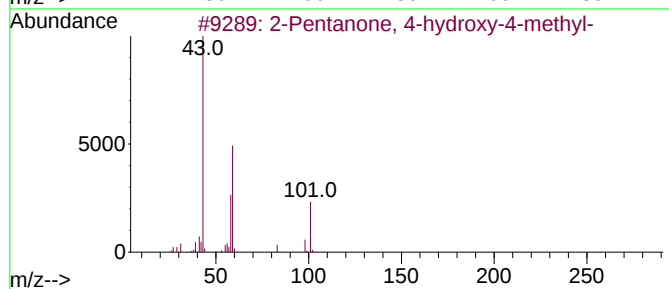
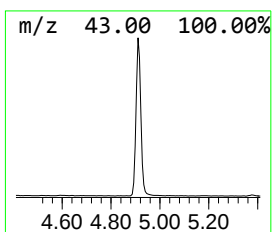
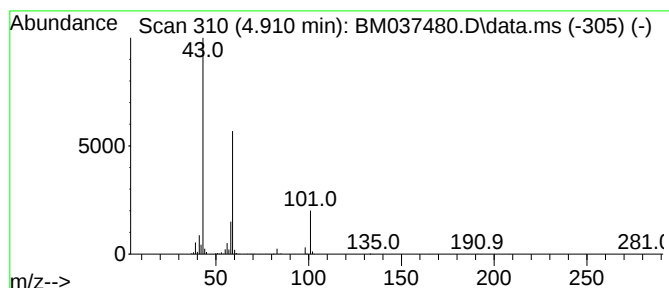
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	26.00 ng	1686180	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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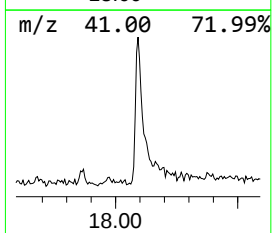
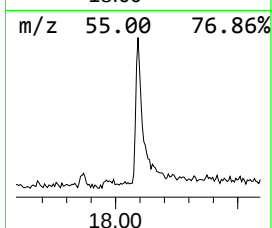
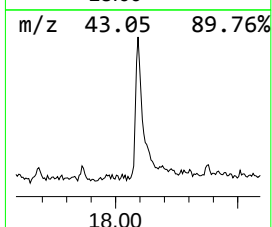
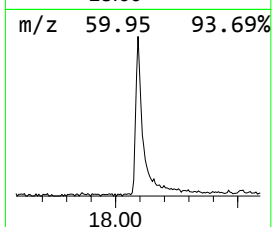
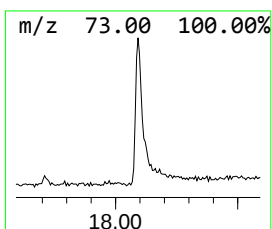
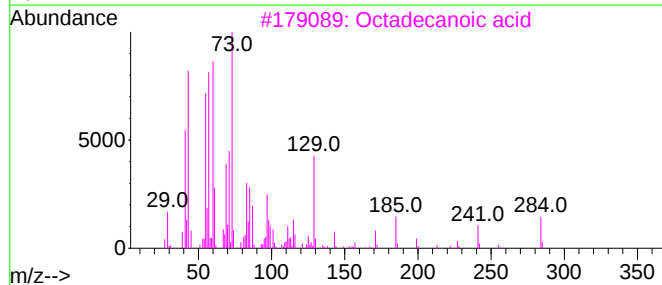
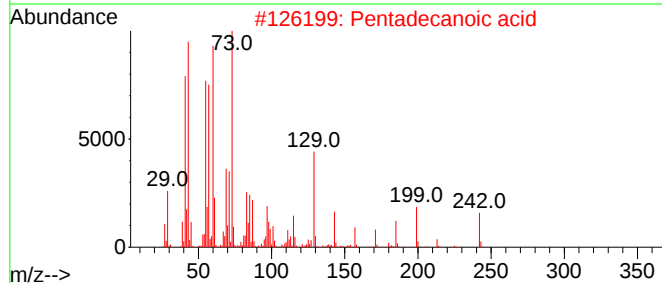
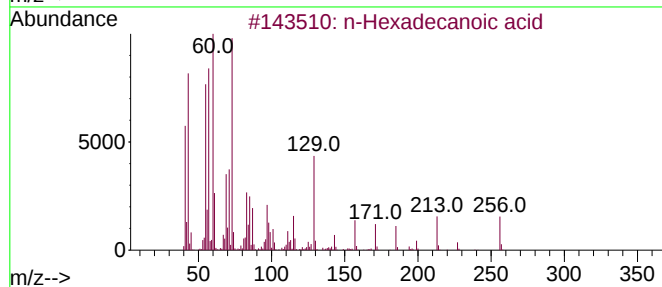
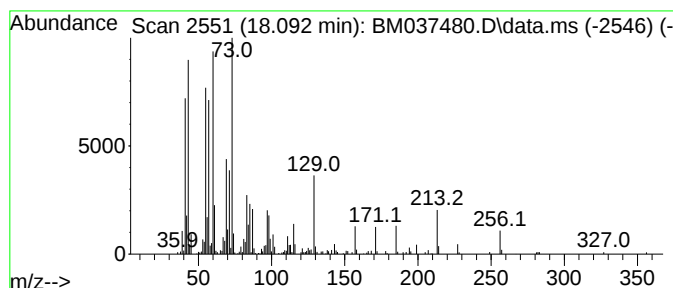
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	3.85 ng	433907	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Octadecanoic acid	284	C18H36O2	000057-11-4	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



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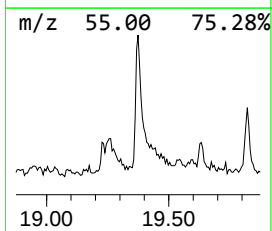
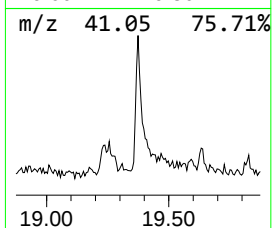
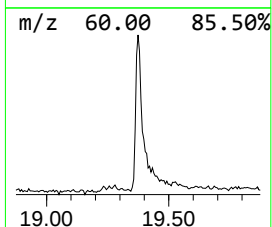
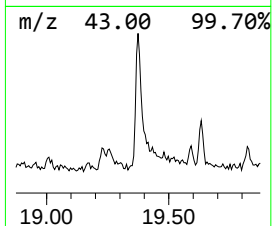
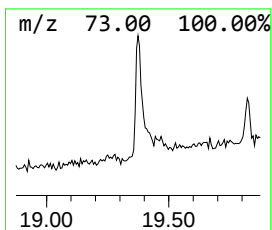
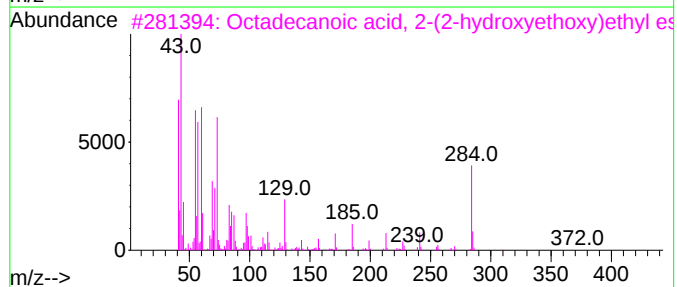
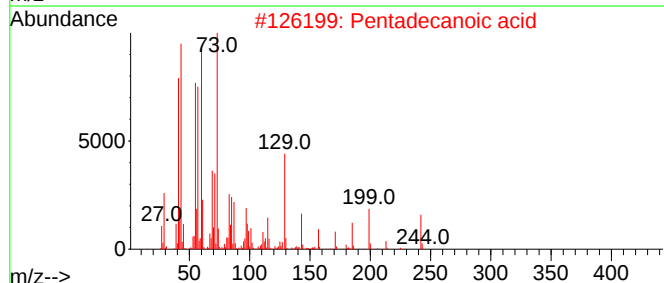
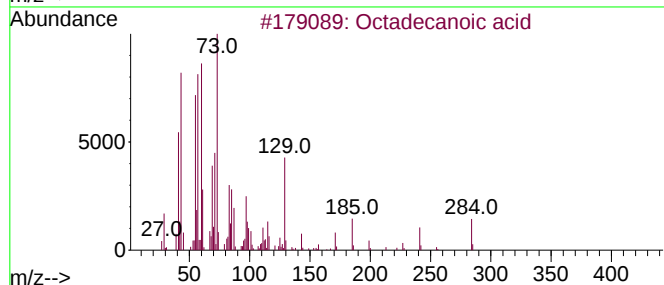
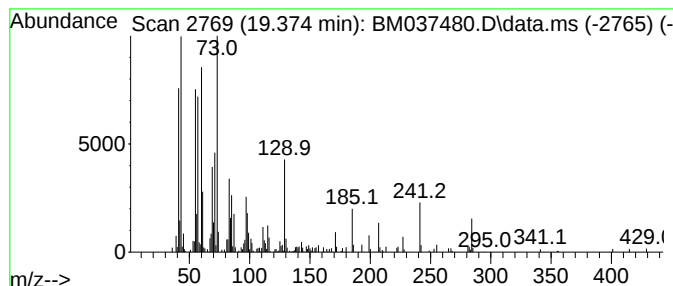
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	2.35 ng	292660	Chrysene-d12	21.380

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	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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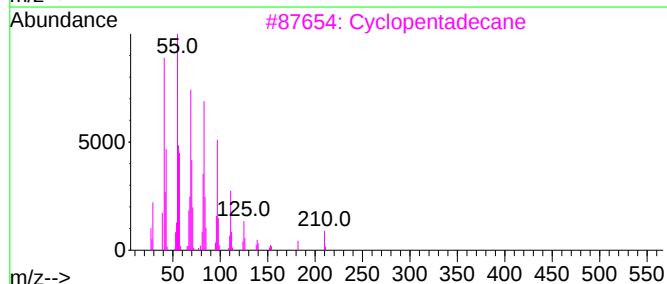
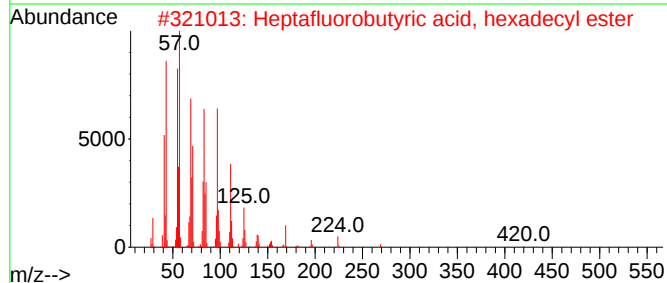
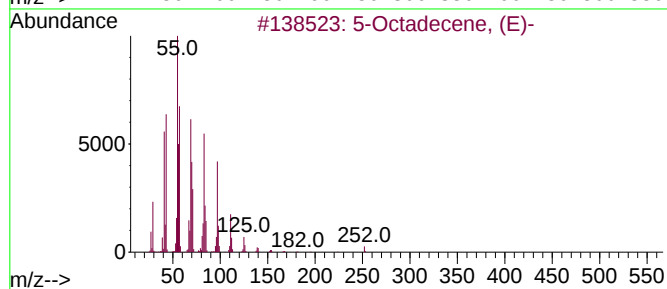
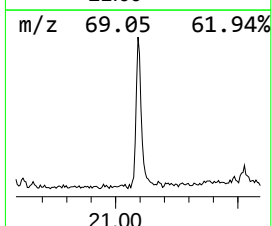
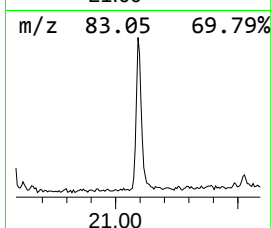
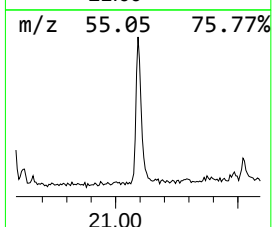
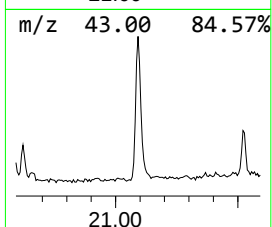
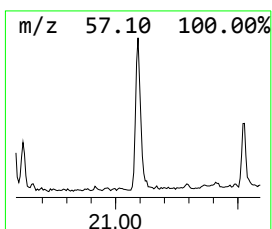
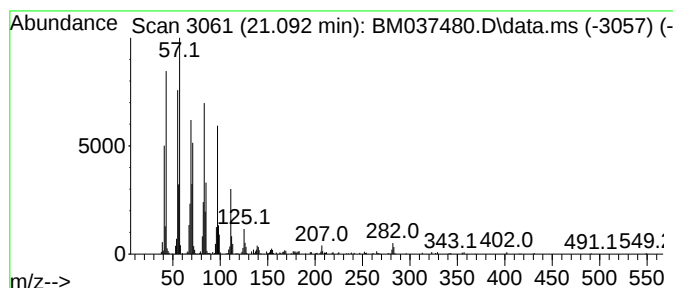
Instrument :
BNA_M
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Octadecene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.092	3.90 ng	487143	Chrysene-d12	21.380	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
Data File : BM037480.D
Acq On : 11 Nov 2022 23:07
Operator : CG/JU
Sample : N5530-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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
1,3-Dioxolane, ...	3.375	2.2	ng	141743	1	7.804	1297070	20.0
3-Penten-2-one,...	4.299	2.7	ng	173887	1	7.804	1297070	20.0
2-Pentanone, 4-...	4.910	26.0	ng	1686180	1	7.804	1297070	20.0
n-Hexadecanoic ...	18.092	3.9	ng	433907	4	17.192	2254730	20.0
Octadecanoic acid	19.374	2.4	ng	292660	5	21.380	2495060	20.0
5-Octadecene, (E)-	21.092	3.9	ng	487143	5	21.380	2495060	20.0