

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
 Data File : BG055687.D
 Acq On : 18 Nov 2022 12:20
 Operator : CG/JU
 Sample : N5598-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FRAC-TANK-0760533

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_G\Methods\8270-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.685	234	238	247	rBV	16021	24966	1.21%	0.194%
2	5.308	337	344	352	rBV	163557	262498	12.68%	2.036%
3	5.784	418	425	434	rVB	610748	978056	47.24%	7.586%
4	7.400	690	700	709	rBV	577906	1012380	48.90%	7.852%
5	8.252	838	845	852	rVB	118691	199779	9.65%	1.550%
6	9.421	1035	1044	1054	rBV	351980	612890	29.60%	4.754%
7	10.831	1277	1284	1296	rBV2	33603	64631	3.12%	0.501%
8	11.078	1318	1326	1333	rBV	149932	272968	13.18%	2.117%
9	13.499	1730	1738	1745	rBV	856113	1323605	63.93%	10.266%
10	14.368	1858	1886	1889	rBV7	72853	422931	20.43%	3.280%
11	14.873	1966	1972	1985	rVB	245692	404333	19.53%	3.136%
12	16.354	2218	2224	2237	rBV	801535	1258916	60.80%	9.764%
13	17.611	2433	2438	2445	rVB	317446	479163	23.14%	3.717%
14	19.727	2790	2798	2819	rVB	391552	1292732	62.44%	10.027%
15	19.991	2839	2843	2851	rVB	68471	106761	5.16%	0.828%
16	20.202	2873	2879	2884	rBV	1535448	2070500	100.00%	16.059%
17	20.743	2966	2971	2979	rBV2	76363	144308	6.97%	1.119%
18	20.984	3009	3012	3015	rVB2	32439	35669	1.72%	0.277%
19	21.513	3096	3102	3112	rVB2	117897	248556	12.00%	1.928%
20	21.912	3164	3170	3177	rVB	331203	562482	27.17%	4.363%
21	22.083	3196	3199	3203	rVB2	39075	52393	2.53%	0.406%
22	22.382	3244	3250	3258	rVB	76452	184785	8.92%	1.433%
23	22.723	3305	3308	3313	rVB2	42907	65294	3.15%	0.506%
24	23.405	3418	3424	3430	rBV	71847	163144	7.88%	1.265%
25	25.326	3743	3751	3763	rVB2	221375	649047	31.35%	5.034%

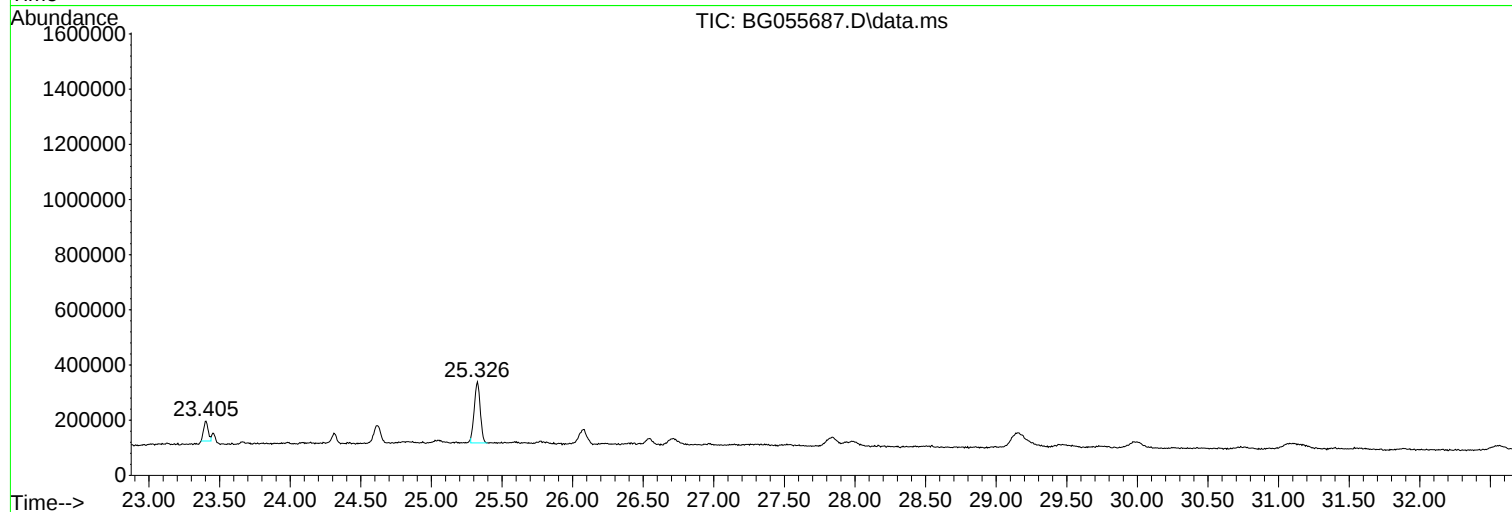
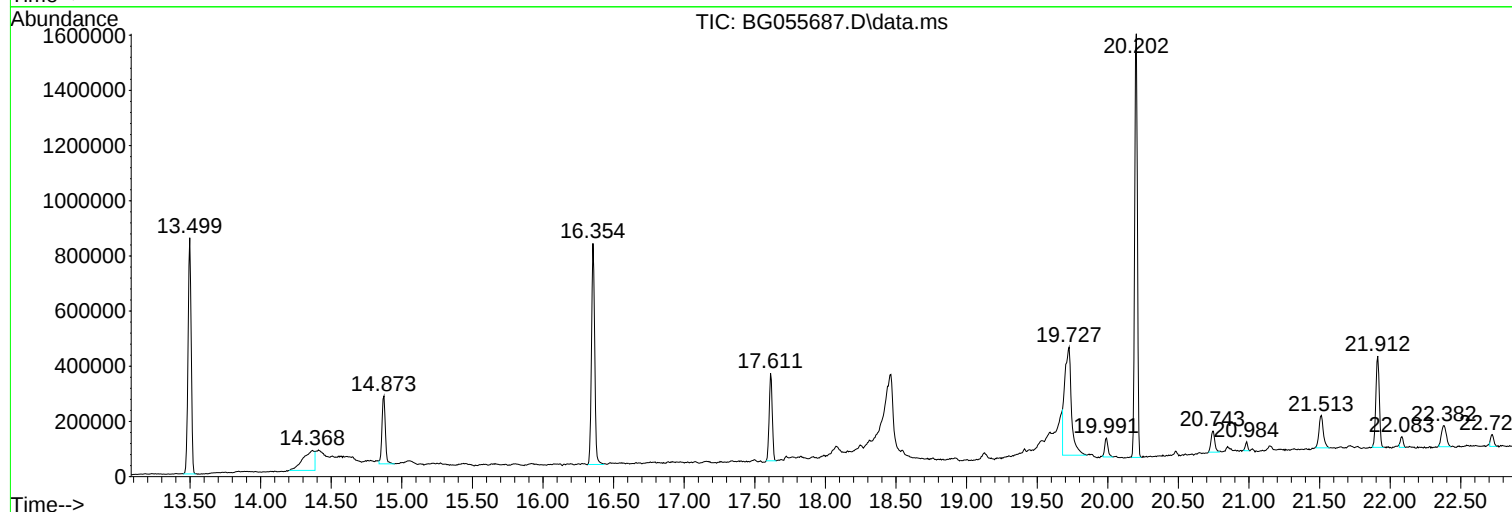
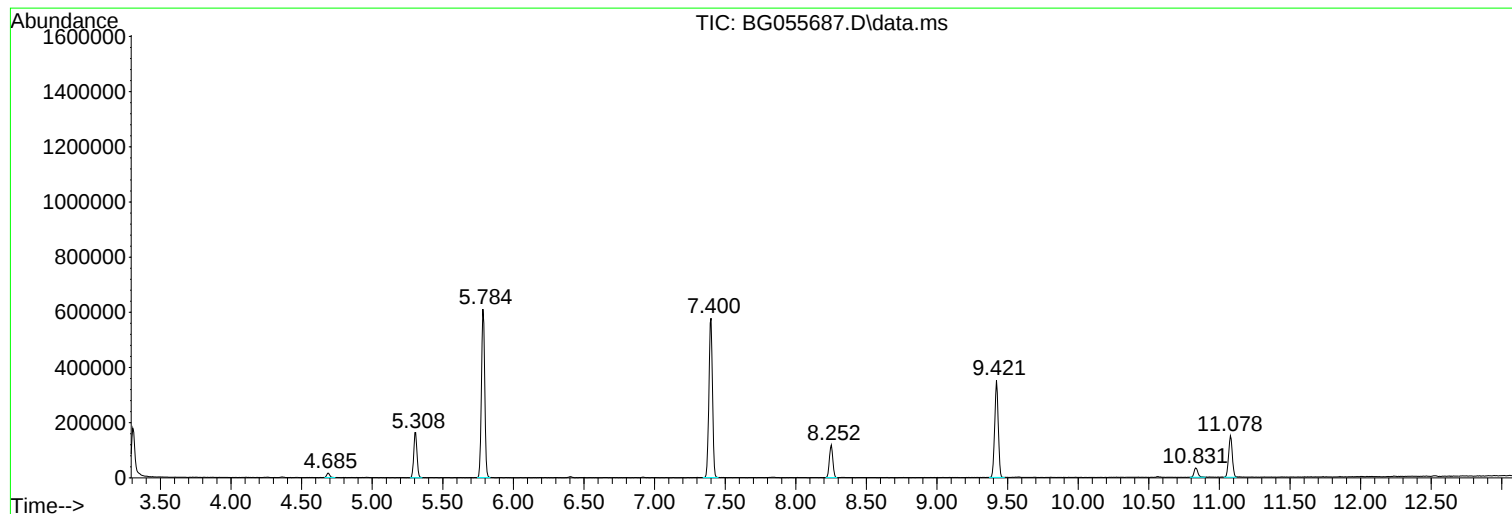
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Instrument :
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ClientSampleId :
FRAC-TANK-0760533

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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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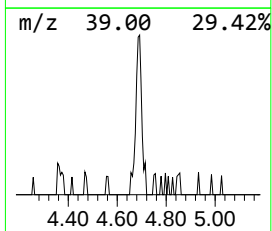
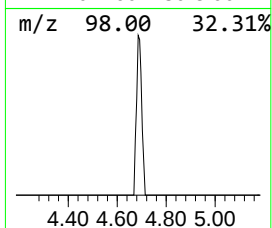
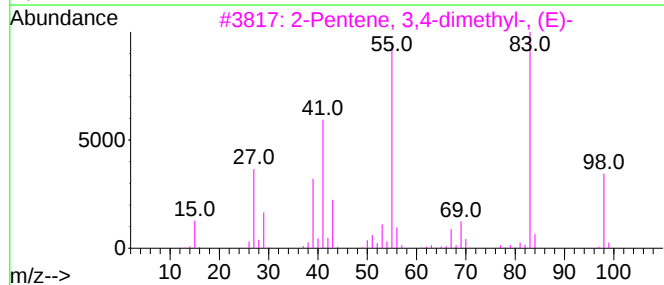
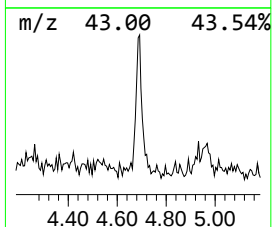
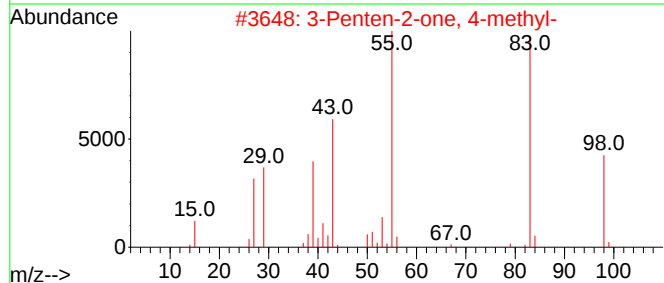
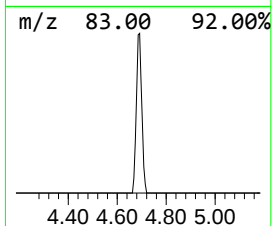
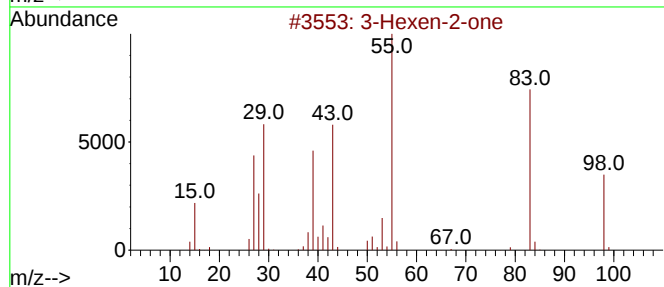
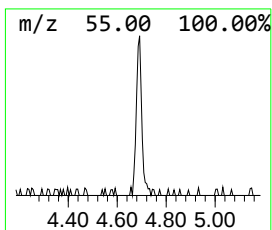
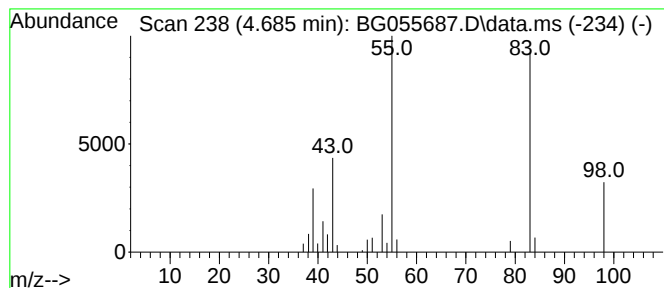
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.685	2.50 ng	24966	1,4-Dichlorobenzene-d4	8.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	90
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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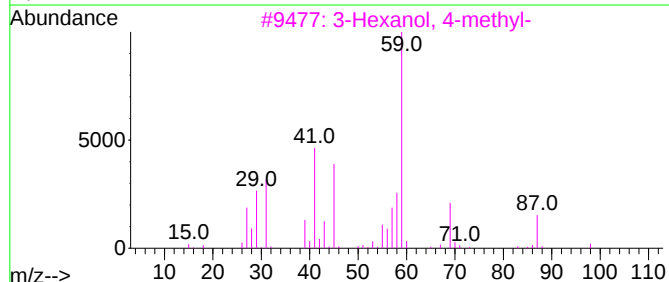
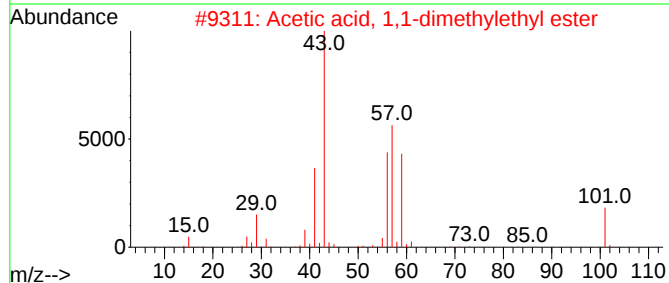
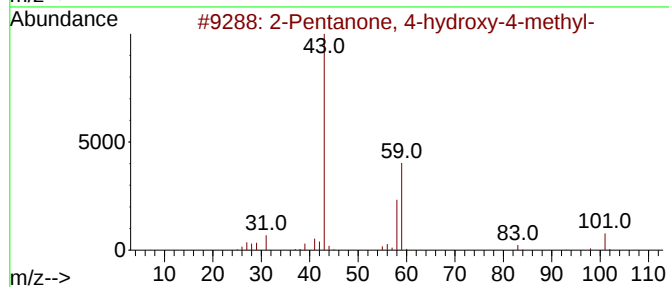
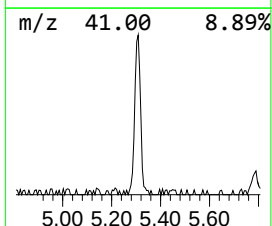
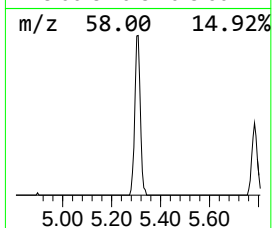
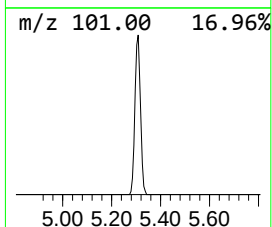
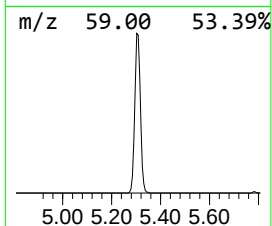
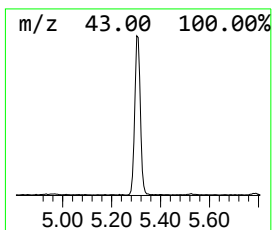
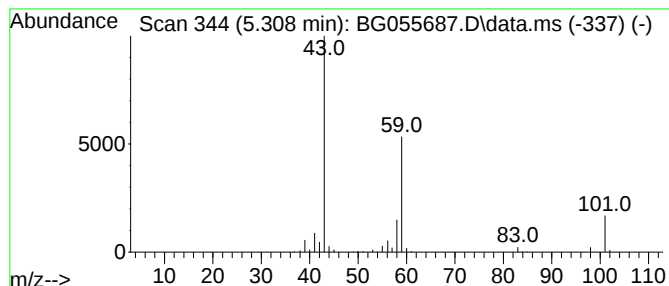
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.308	26.28 ng	262498	1,4-Dichlorobenzene-d4	8.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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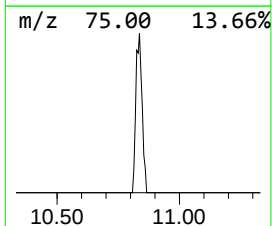
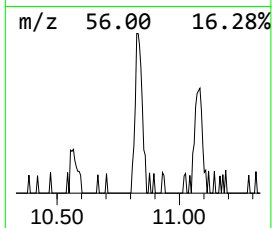
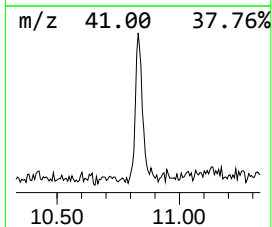
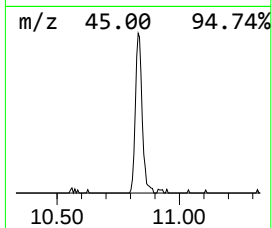
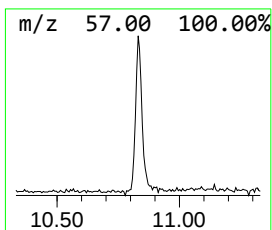
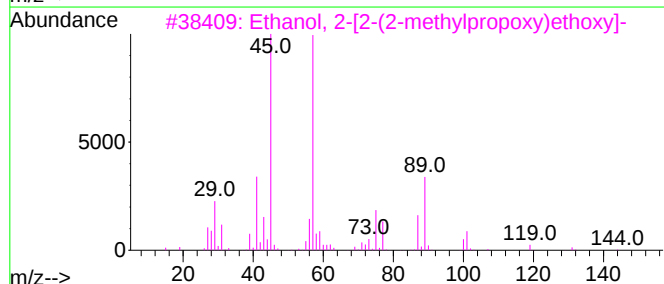
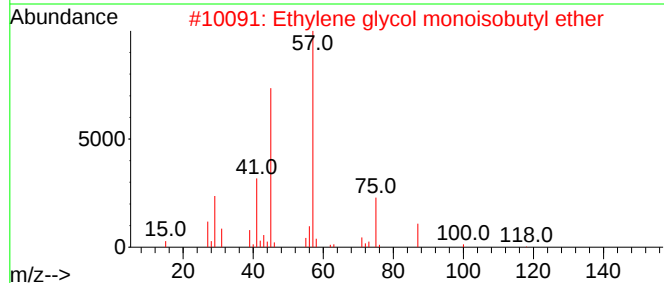
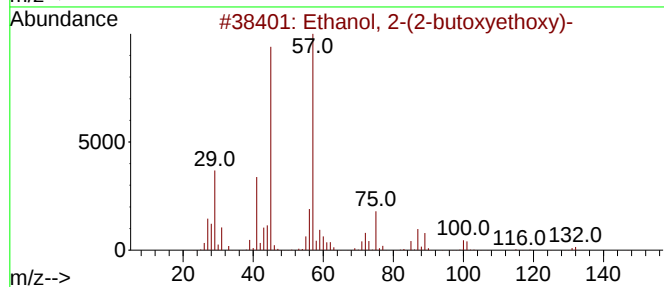
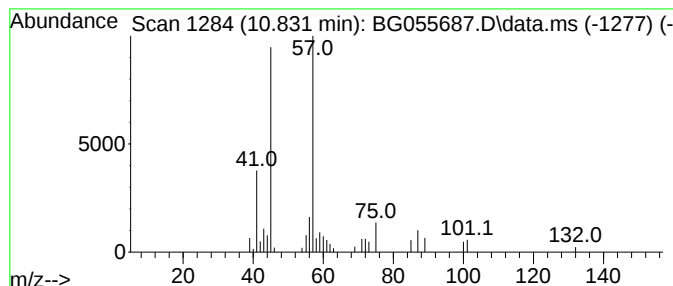
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.831	4.74 ng	64631	Naphthalene-d8	11.078

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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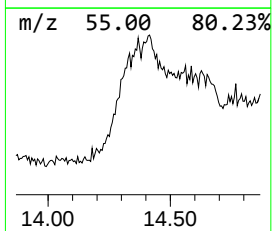
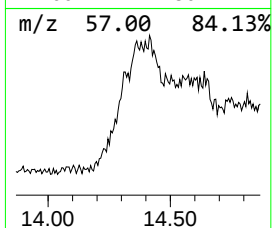
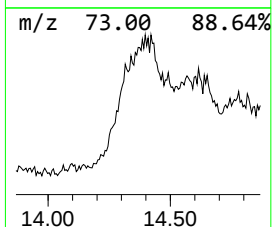
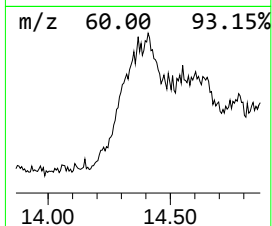
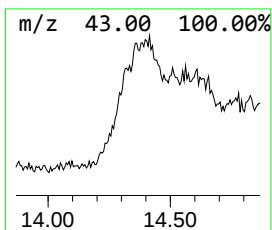
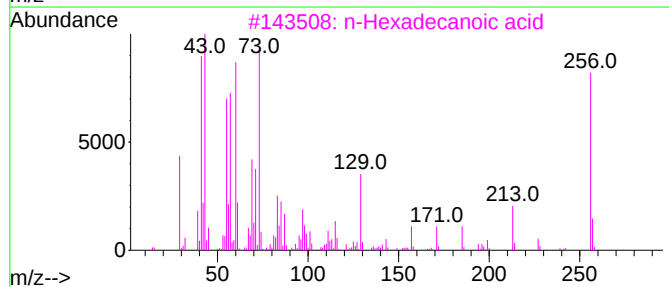
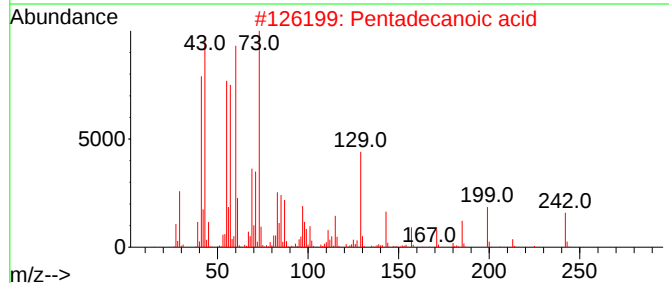
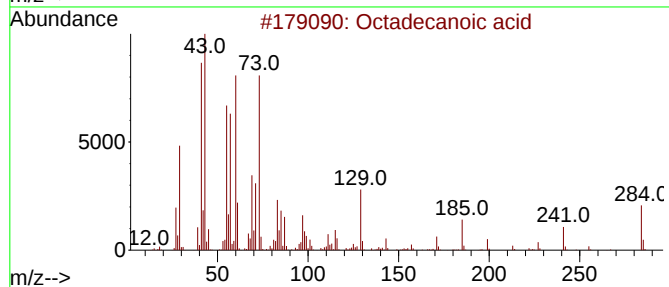
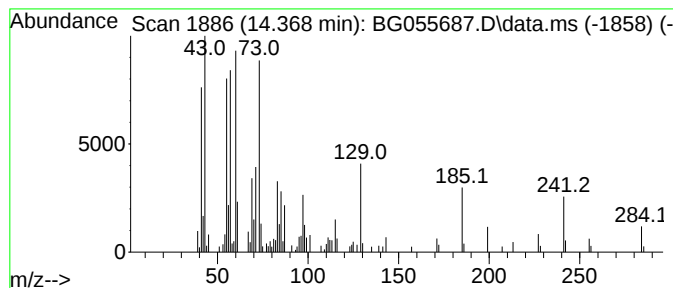
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	20.92 ng	422931	Acenaphthene-d10	14.873

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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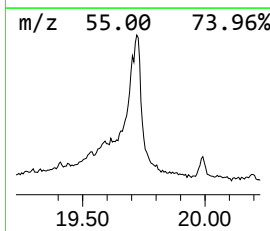
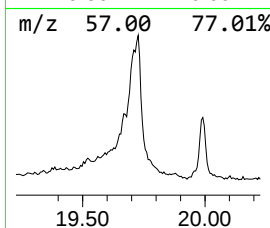
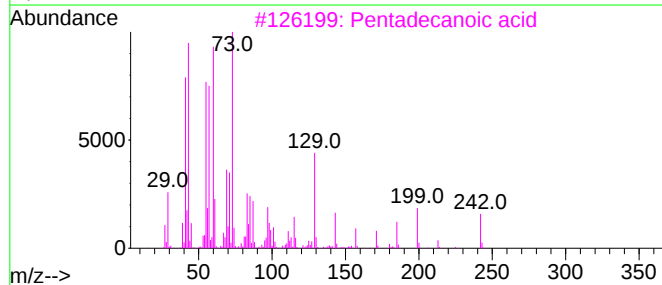
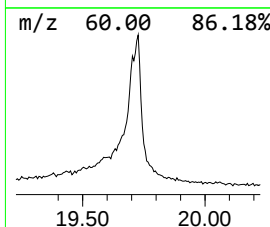
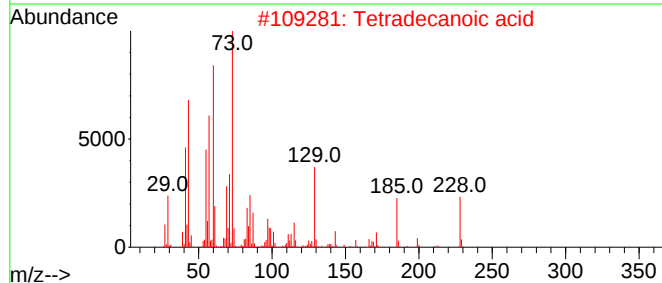
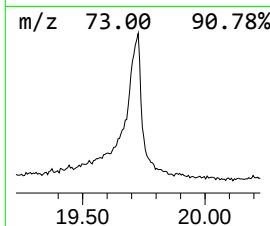
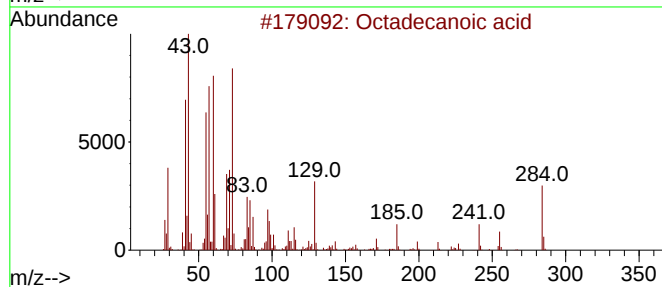
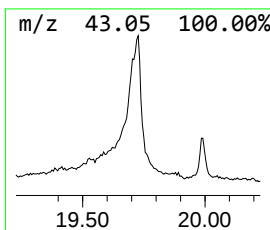
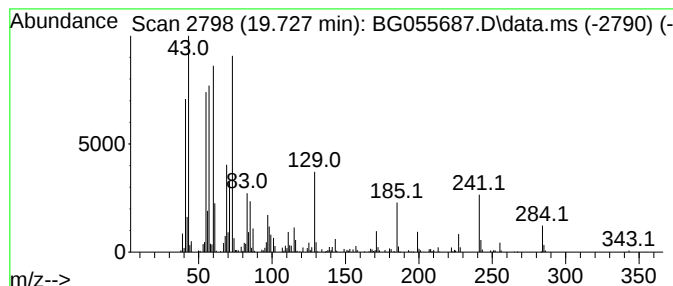
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetradecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.727	53.96 ng	1292730	Phenanthrene-d10	17.611

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4			Undecanoic acid	186	C11H22O2	000112-37-8	53
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



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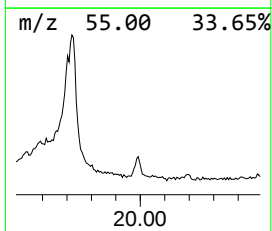
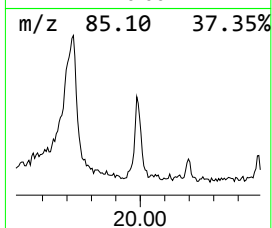
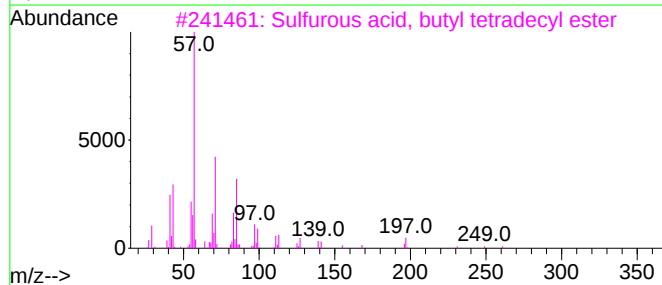
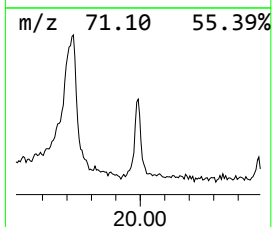
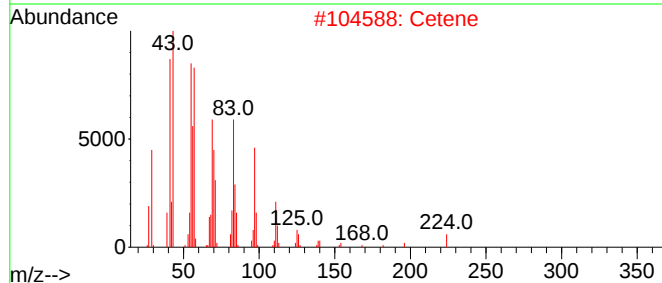
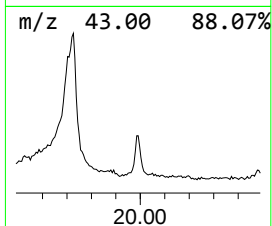
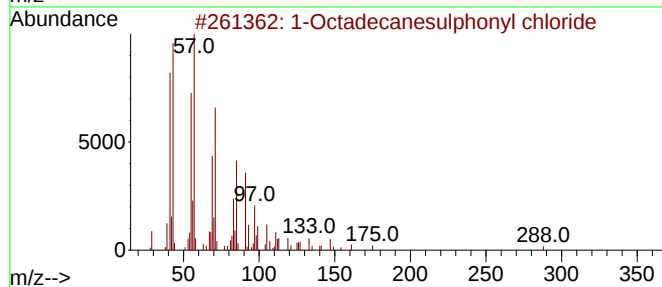
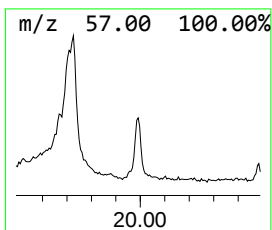
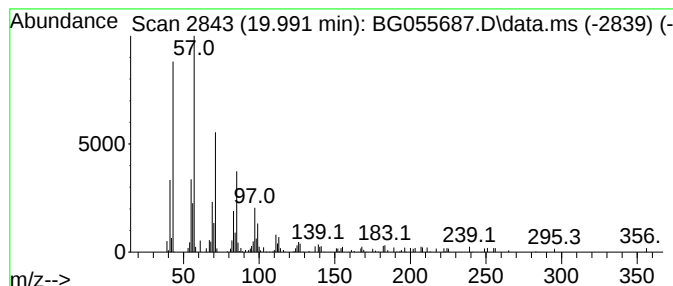
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.991	3.80 ng	106761	Chrysene-d12	21.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2			Cetene	224	C16H32	000629-73-2	86
3			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	83
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	72
5			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055687.D
Acq On : 18 Nov 2022 12:20
Operator : CG/JU
Sample : N5598-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FRAC-TANK-0760533

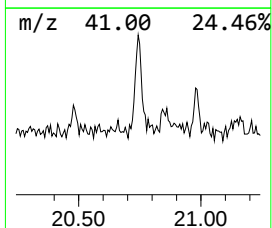
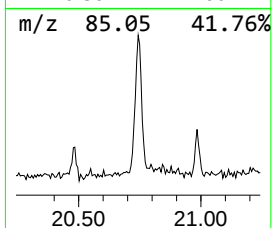
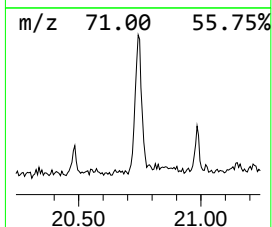
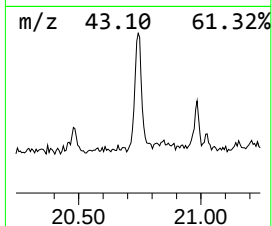
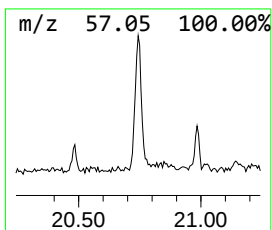
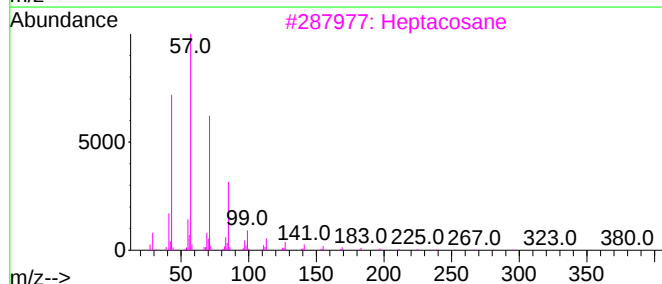
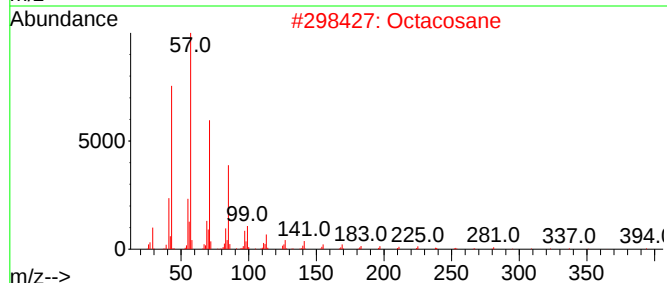
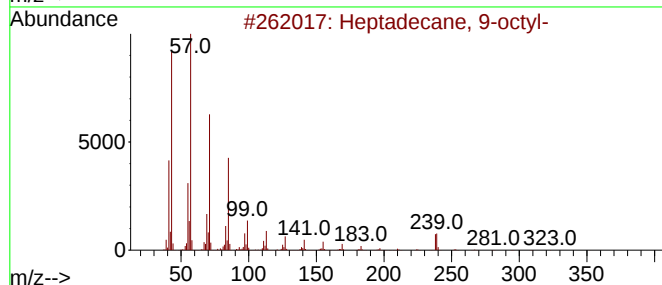
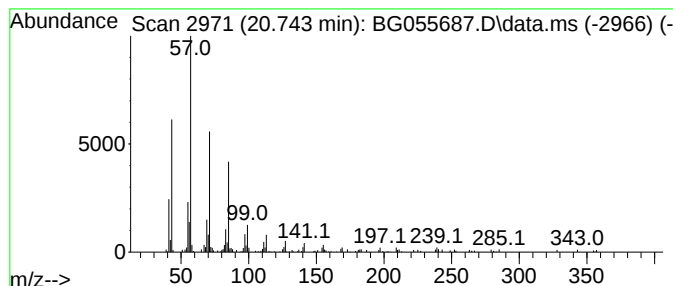
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.743	5.13 ng	144308	Chrysene-d12	21.912

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2		Octacosane	394	C28H58	000630-02-4	87
3		Heptacosane	380	C27H56	000593-49-7	87
4		Hexadecane	226	C16H34	000544-76-3	83
5		Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055687.D
Acq On : 18 Nov 2022 12:20
Operator : CG/JU
Sample : N5598-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FRAC-TANK-0760533

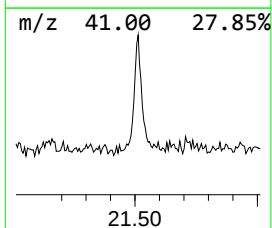
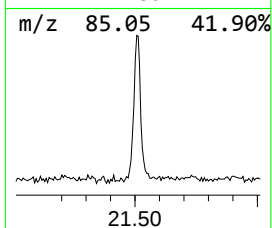
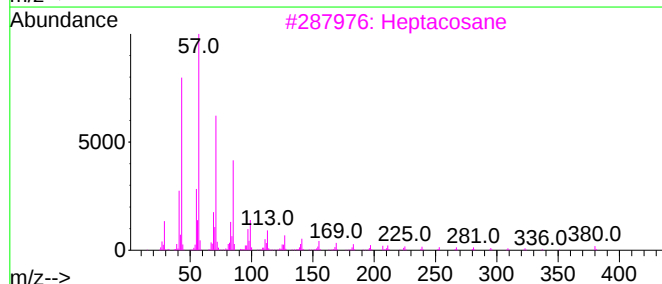
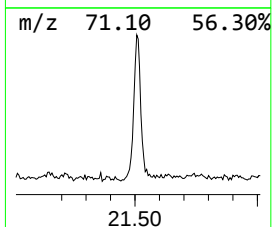
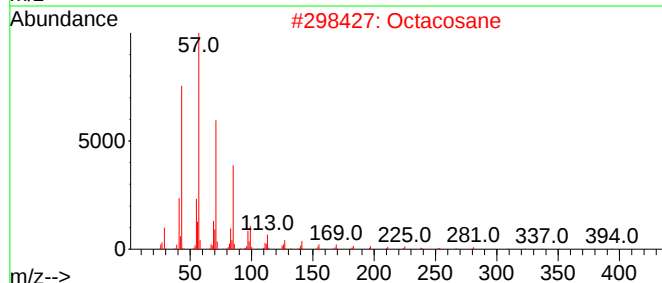
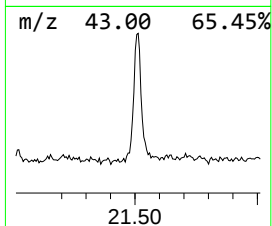
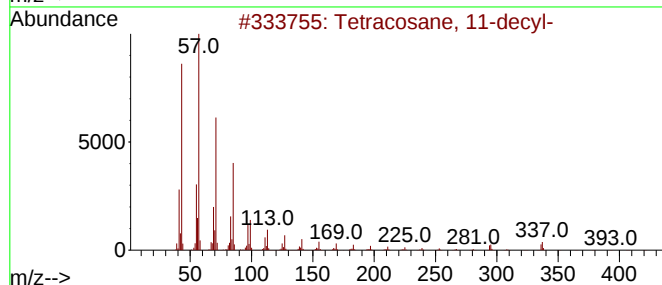
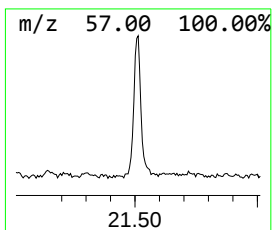
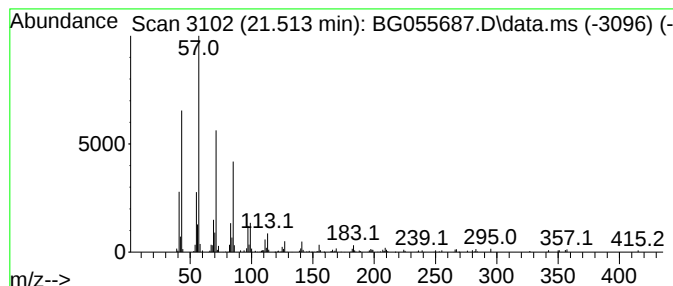
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane, 11-decyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.513	8.84 ng	248556	Chrysene-d12	21.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055687.D
Acq On : 18 Nov 2022 12:20
Operator : CG/JU
Sample : N5598-01
Misc :
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Instrument :
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ClientSampleId :
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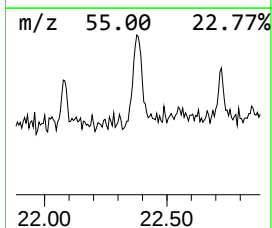
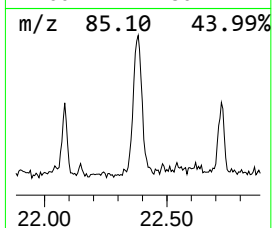
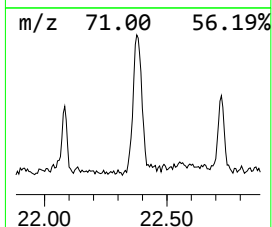
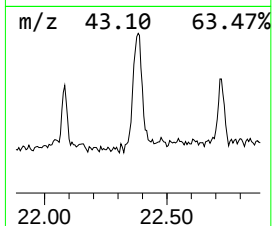
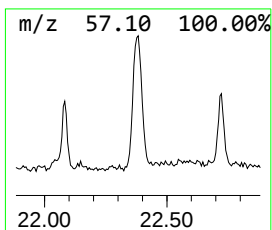
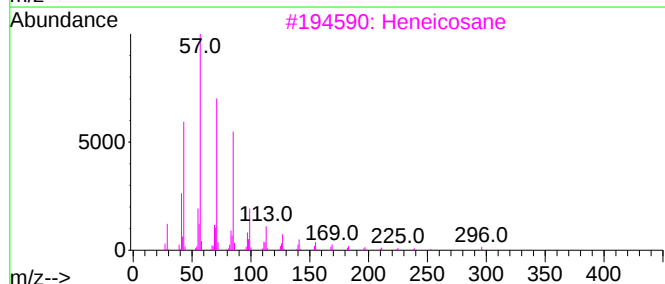
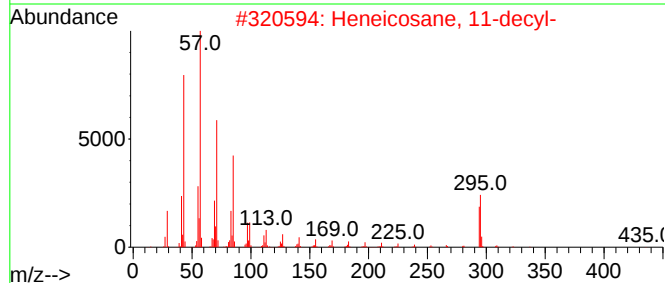
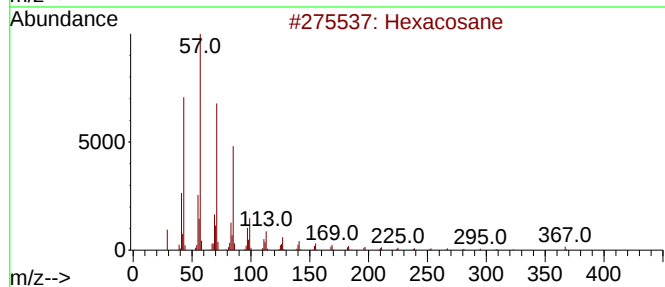
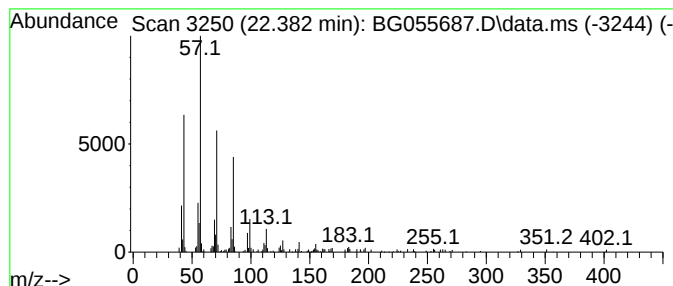
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.382	6.57 ng	184785	Chrysene-d12	21.912

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	90
2		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055687.D
Acq On : 18 Nov 2022 12:20
Operator : CG/JU
Sample : N5598-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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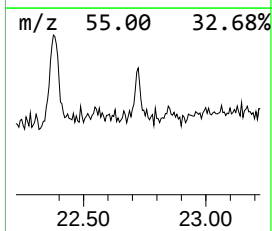
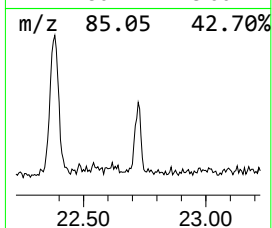
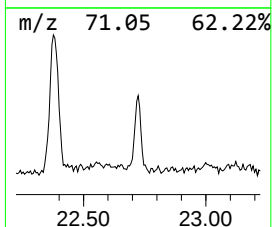
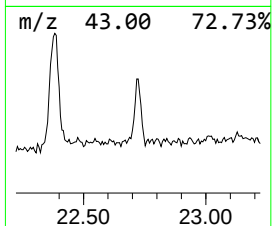
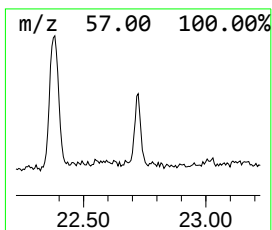
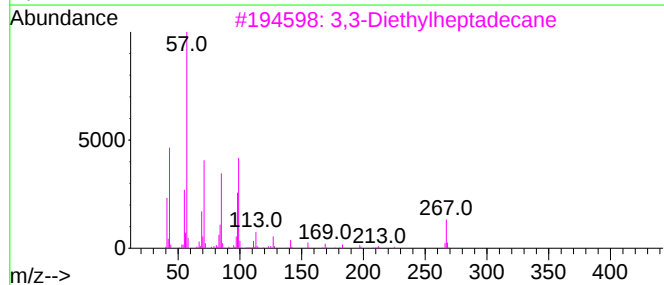
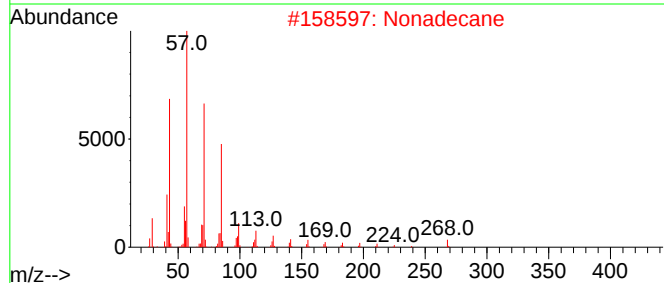
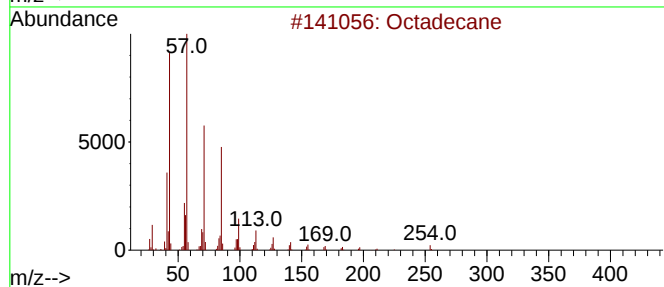
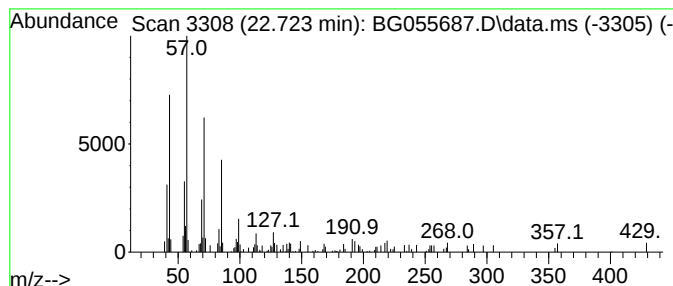
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.723	2.32 ng	65294	Chrysene-d12	21.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	92
2			Nonadecane	268	C19H40	000629-92-5	89
3			3,3-Diethylheptadecane	296	C21H44	1000360-41-6	64
4			Docosane	310	C22H46	000629-97-0	62
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055687.D
Acq On : 18 Nov 2022 12:20
Operator : CG/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FRAC-TANK-0760533

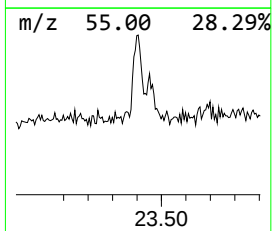
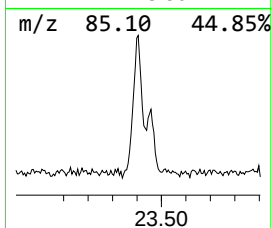
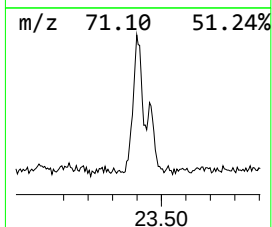
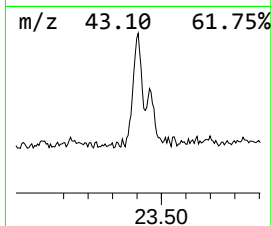
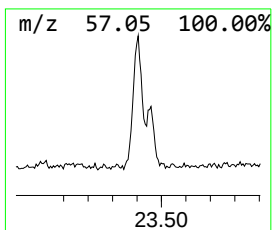
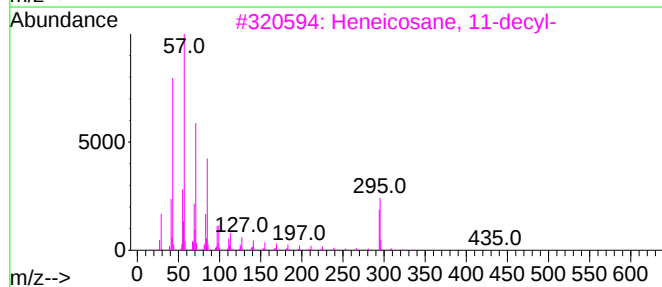
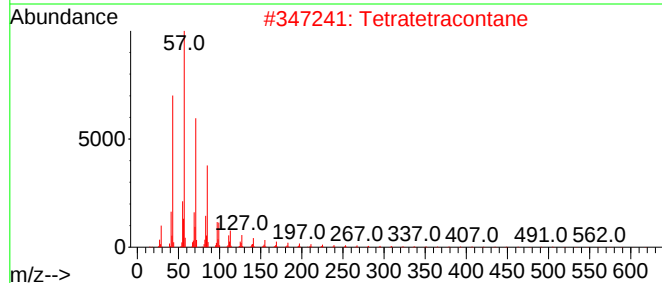
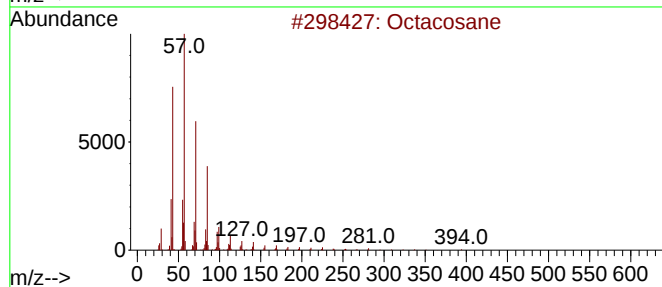
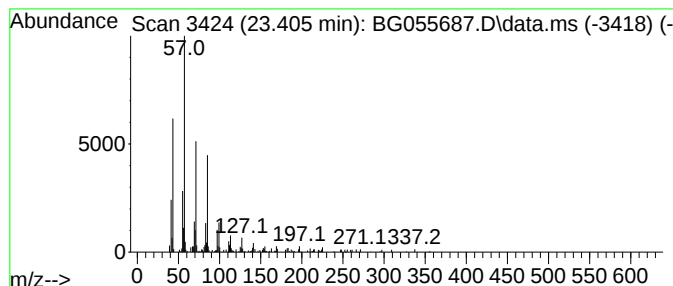
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.405	5.80 ng	163144	Chrysene-d12	21.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
4			Tetracosane	338	C24H50	000646-31-1	87
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
Data File : BG055687.D
Acq On : 18 Nov 2022 12:20
Operator : CG/JU
Sample : N5598-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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
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2-Pentanone, 4-...	5.308	26.3	ng	262498	1	8.252	199779	20.0
Ethanol, 2-(2-b...	10.831	4.7	ng	64631	2	11.078	272968	20.0
Octadecanoic acid	14.368	20.9	ng	422931	3	14.873	404333	20.0
Tetradecanoic acid	19.727	54.0	ng	1292730	4	17.611	479163	20.0
1-Octadecanesul...	19.991	3.8	ng	106761	5	21.912	562482	20.0
Heptadecane, 9-...	20.743	5.1	ng	144308	5	21.912	562482	20.0
Tetracosane, 11...	21.513	8.8	ng	248556	5	21.912	562482	20.0
Hexacosane	22.382	6.6	ng	184785	5	21.912	562482	20.0
Octadecane	22.723	2.3	ng	65294	5	21.912	562482	20.0
Octacosane	23.405	5.8	ng	163144	5	21.912	562482	20.0