

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
 Data File : BM041205.D
 Acq On : 01 Aug 2023 02:05
 Operator : MA/JU
 Sample : 03741-04
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B-P24A

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-BM072823.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041205.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	364	371	384	rBV	2724944	3823450	56.36%	8.866%
2	6.981	637	645	662	rBV	2559576	4077360	60.11%	9.455%
3	7.563	739	744	757	rVB	55286	109177	1.61%	0.253%
4	7.798	776	784	793	rBV	717269	1085078	16.00%	2.516%
5	7.887	793	799	815	rVV	131790	291809	4.30%	0.677%
6	8.316	866	872	884	rVB	152868	262258	3.87%	0.608%
7	8.975	976	984	999	rBV	1600861	2593841	38.24%	6.015%
8	10.410	1220	1228	1245	rBV	484660	1072557	15.81%	2.487%
9	10.604	1254	1261	1268	rBV	908678	1463460	21.57%	3.393%
10	11.645	1432	1438	1445	rBV	127160	220829	3.26%	0.512%
11	11.716	1445	1450	1459	rVB	57108	93749	1.38%	0.217%
12	13.080	1675	1682	1693	rBV	3941665	5493748	80.99%	12.739%
13	13.927	1818	1826	1835	rBV	178755	256563	3.78%	0.595%
14	14.463	1911	1917	1924	rBV	1286351	1816571	26.78%	4.212%
15	15.963	2165	2172	2181	rBV	3320459	4410866	65.02%	10.228%
16	17.221	2380	2386	2396	rBV	1524855	2074603	30.58%	4.811%
17	18.004	2514	2519	2526	rBV5	39785	95521	1.41%	0.221%
18	18.121	2534	2539	2550	rBV	740790	1101376	16.24%	2.554%
19	19.286	2734	2737	2751	rVB	72185	151563	2.23%	0.351%
20	19.403	2753	2757	2770	rBV	153073	270733	3.99%	0.628%
21	19.651	2797	2799	2808	rVB2	37773	71120	1.05%	0.165%
22	19.856	2829	2834	2839	rBV	5839848	6783545	100.00%	15.730%
23	20.539	2947	2950	2957	rBV2	195217	286872	4.23%	0.665%
24	21.127	3046	3050	3060	rVB	579826	821139	12.10%	1.904%
25	21.421	3095	3100	3105	rBV	1765841	2202360	32.47%	5.107%
26	23.791	3497	3503	3513	rVB	1150314	2195494	32.36%	5.091%

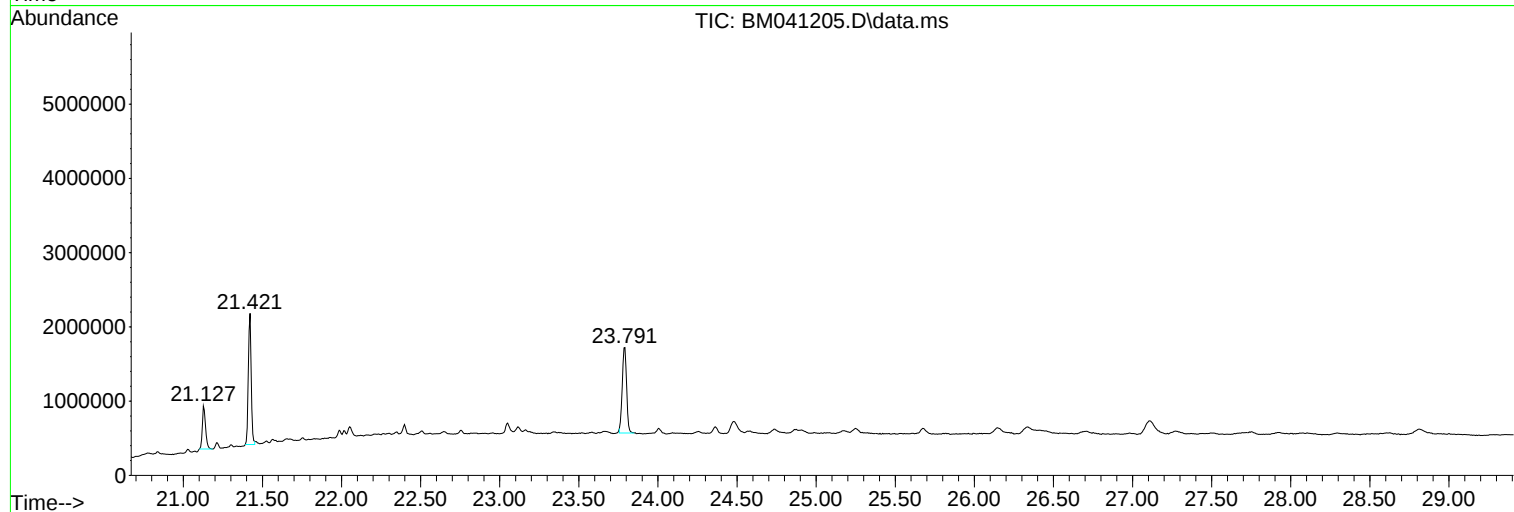
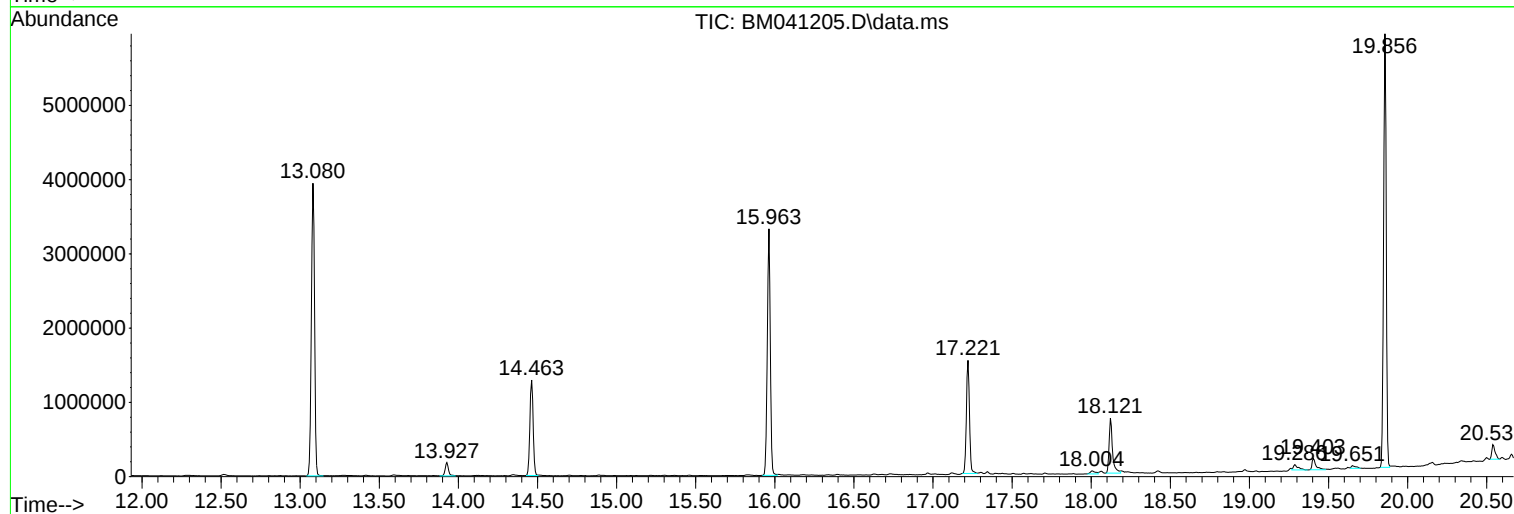
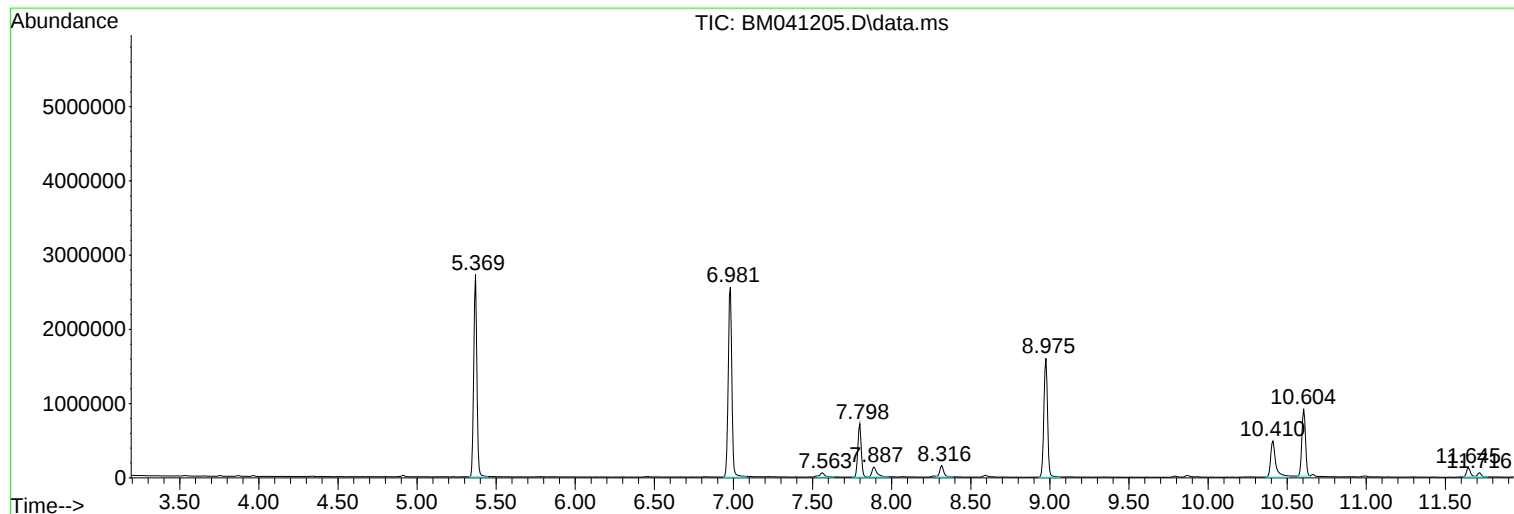
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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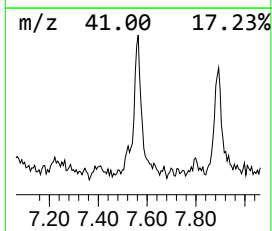
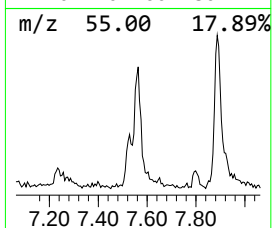
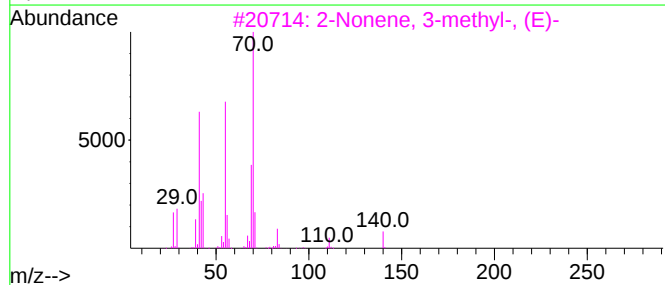
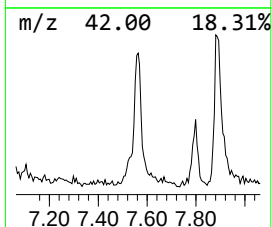
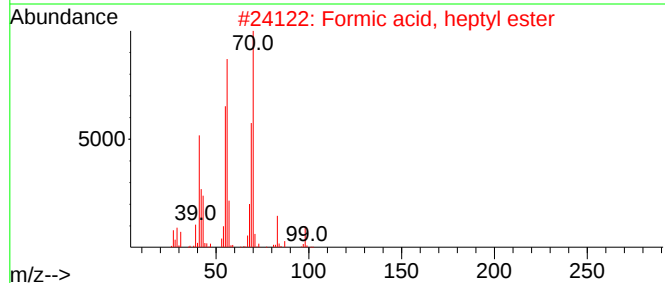
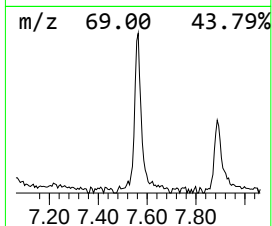
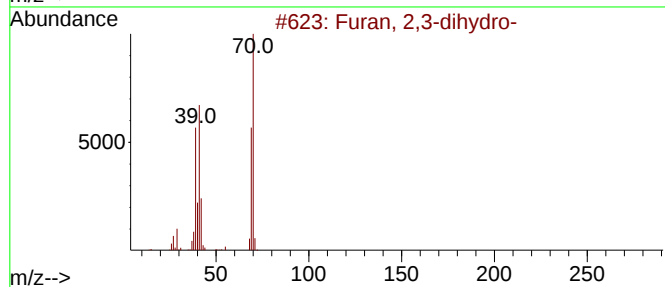
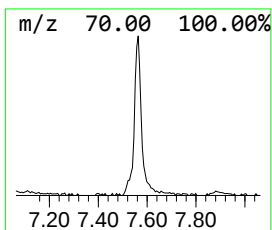
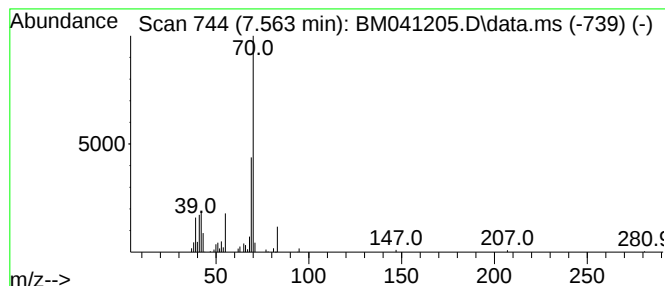
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Furan, 2,3-dihydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	2.01 ng	109177	1,4-Dichlorobenzene-d4	7.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	64
2			Formic acid, heptyl ester	144	C8H16O2	000112-23-2	40
3			2-Nonene, 3-methyl-, (E)-	140	C10H20	017003-99-5	40
4			Aniline, 3-(pyrrolidine-1-sulfon...	226	C10H14N2O2S	1000303-72-7	38
5			Methacrolein	70	C4H6O	000078-85-3	9



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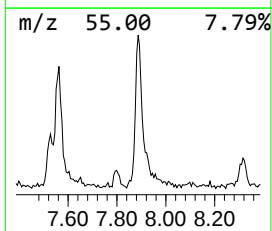
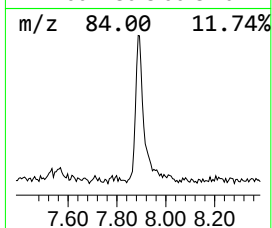
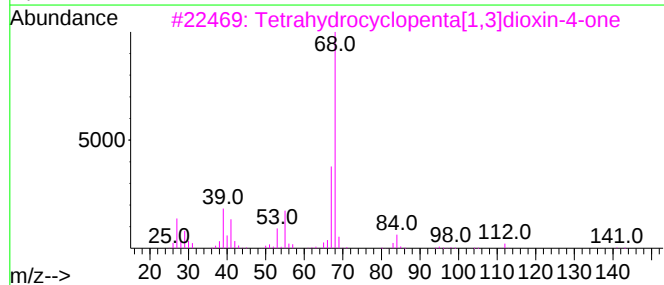
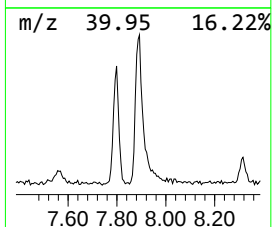
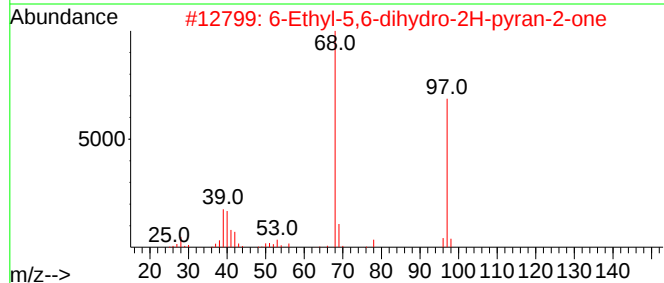
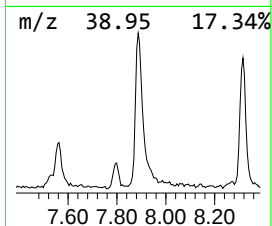
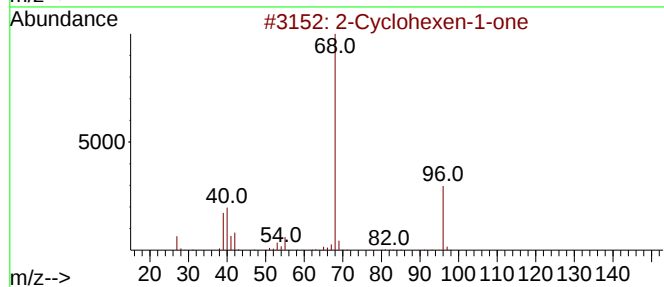
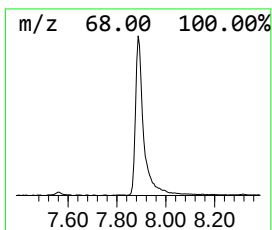
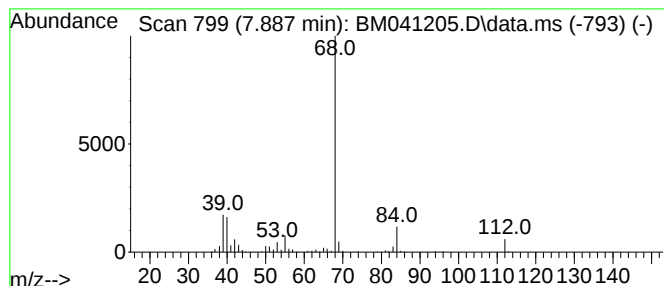
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.887	5.38 ng	291809	1,4-Dichlorobenzene-d4	7.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	64
2			6-Ethyl-5,6-dihydro-2H-pyran-2-one	126	C7H10O2	019895-35-3	59
3			Tetrahydrocyclopenta[1,3]dioxin-...	142	C7H10O3	124898-85-7	39
4			3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	38
5			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	17



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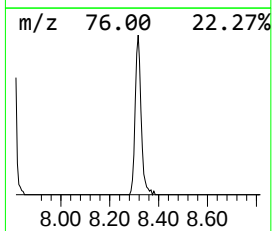
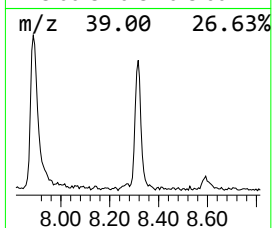
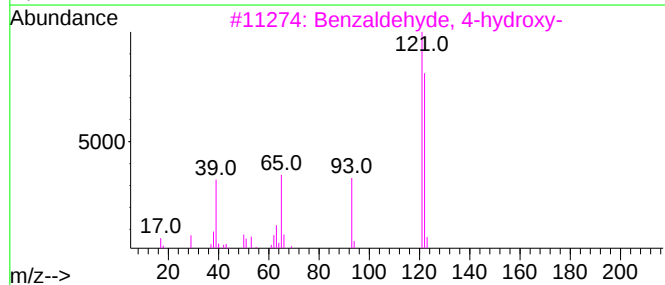
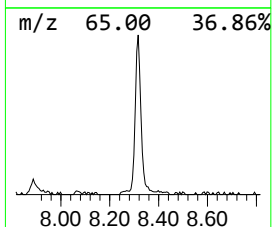
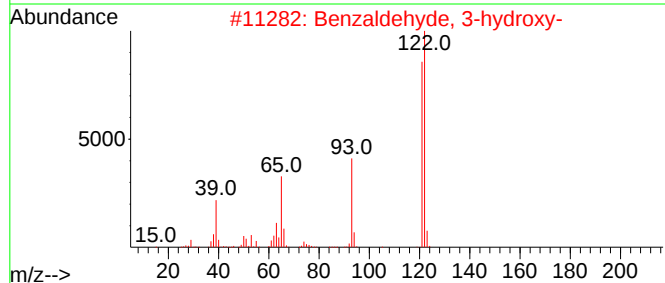
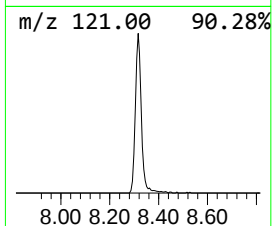
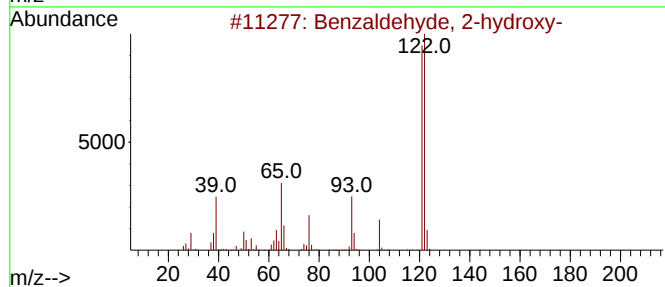
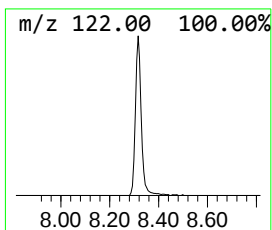
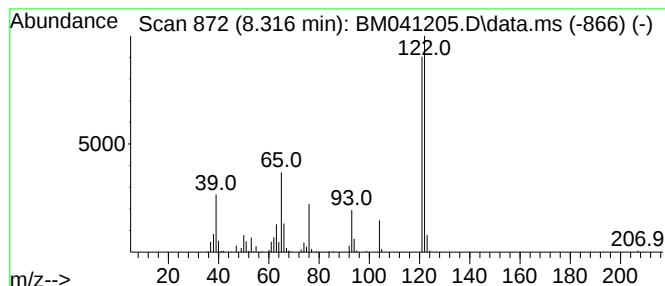
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzaldehyde, 2-hydroxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.316	4.83 ng	262258	1,4-Dichlorobenzene-d4	7.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	97
2			Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	90
3			Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	90
4			Propanoic acid, 3-chloro-, 4-for...	212	C10H9ClO3	1010142-41-5	72
5			3-Acetoxybenzaldehyde	164	C9H8O3	034231-78-2	64



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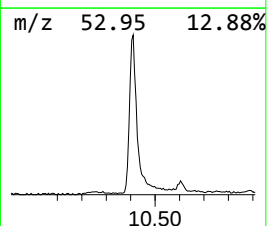
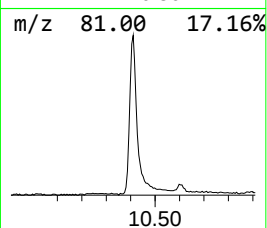
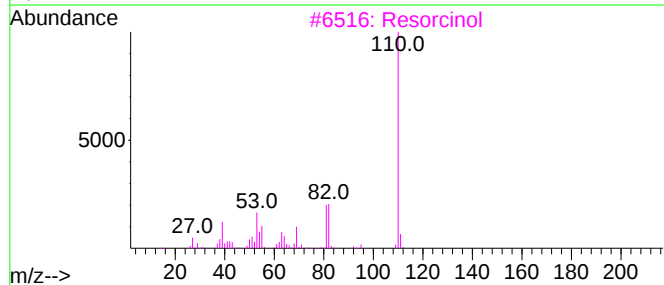
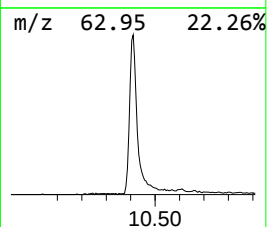
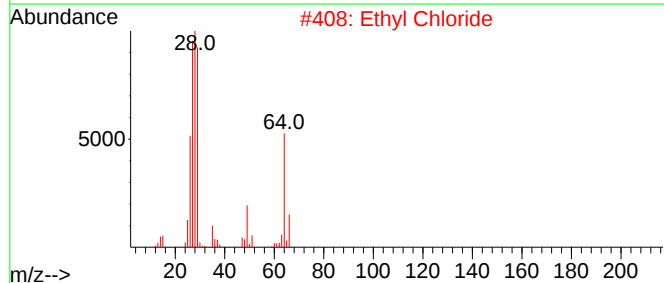
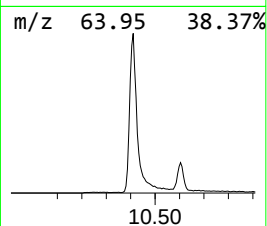
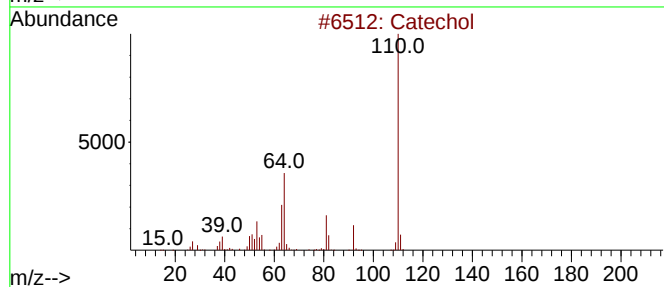
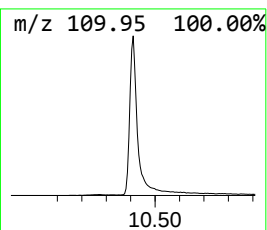
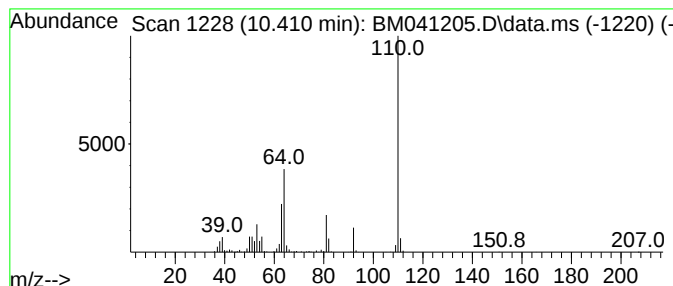
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Peak Number 4 Catechol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.410	14.66 ng	1072560	Naphthalene-d8	10.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Catechol	110	C6H6O2	000120-80-9	96
2			Ethyl Chloride	64	C2H5Cl	000075-00-3	37
3			Resorcinol	110	C6H6O2	000108-46-3	30
4			3(2H)-Pyridazinone, 6-methyl-	110	C5H6N2O	013327-27-0	22
5			2-Furancarboxaldehyde, 5-methyl-	110	C6H6O2	000620-02-0	18



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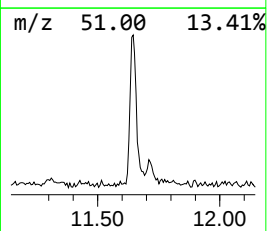
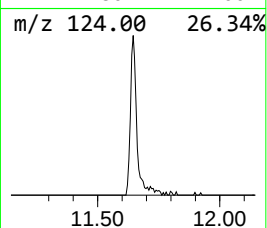
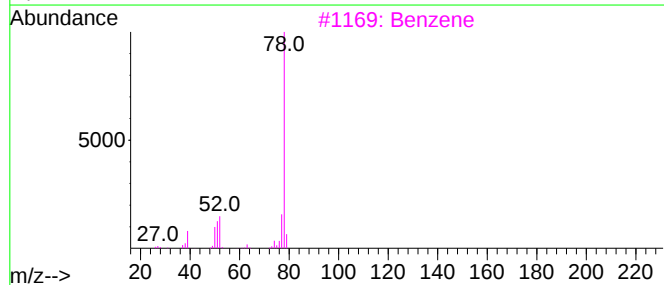
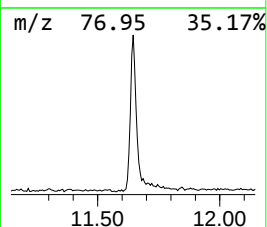
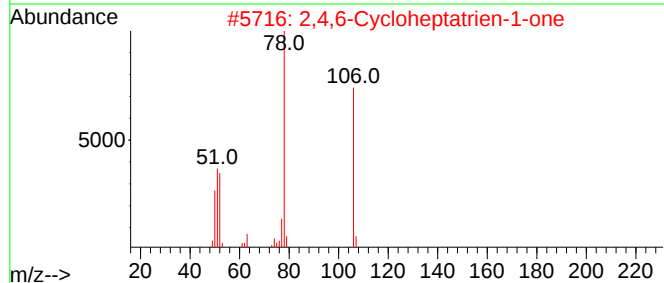
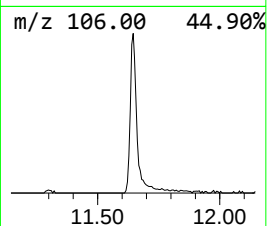
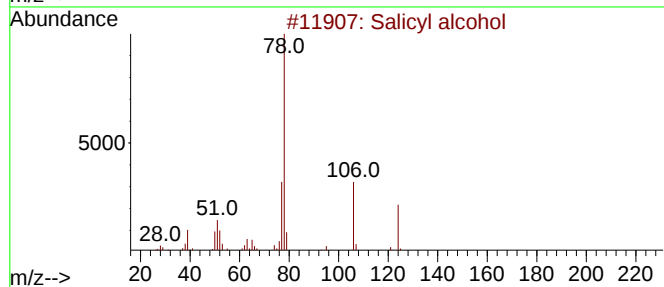
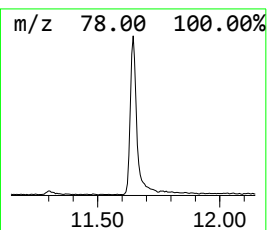
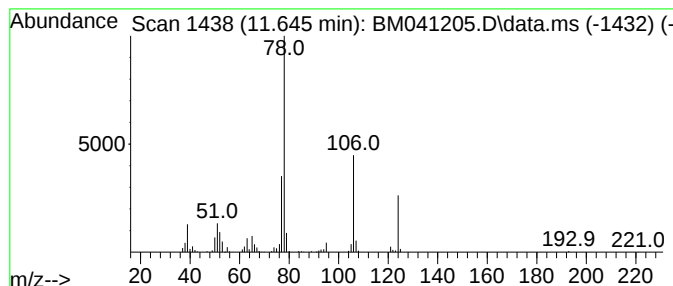
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Peak Number 5 Salicyl alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.645	3.02 ng	220829	Naphthalene-d8	10.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Salicyl alcohol	124	C7H8O2	000090-01-7	91
2			2,4,6-Cycloheptatrien-1-one	106	C7H6O	000539-80-0	90
3			Benzene	78	C6H6	000071-43-2	81
4			2-(Aminomethyl)phenyl acetate	165	C9H11NO2	1010386-75-3	78
5			2-Coumaranone	134	C8H6O2	000553-86-6	78



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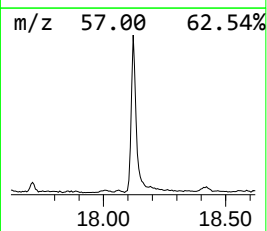
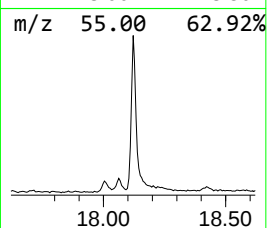
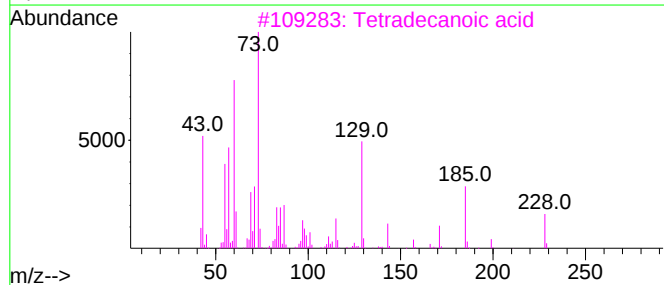
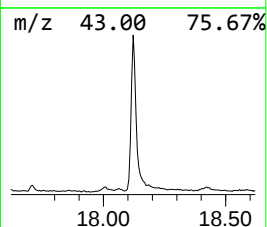
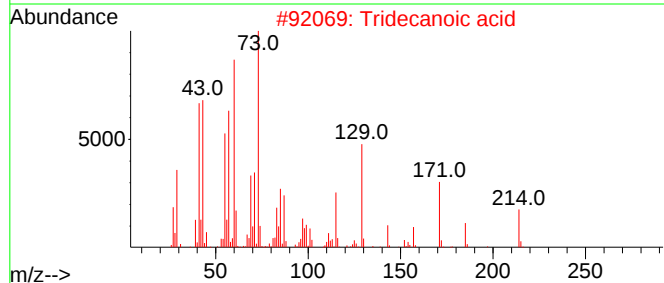
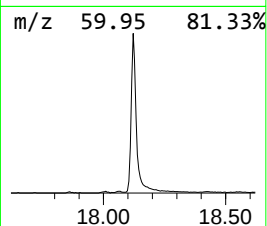
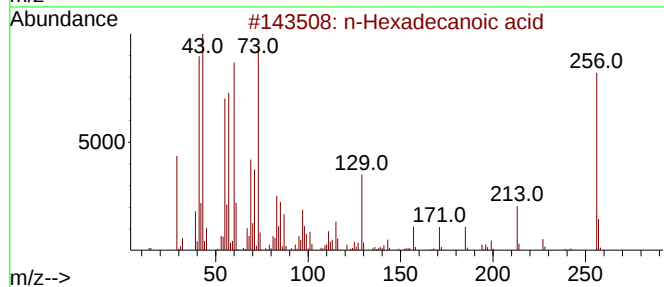
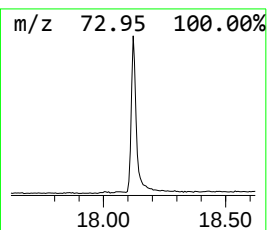
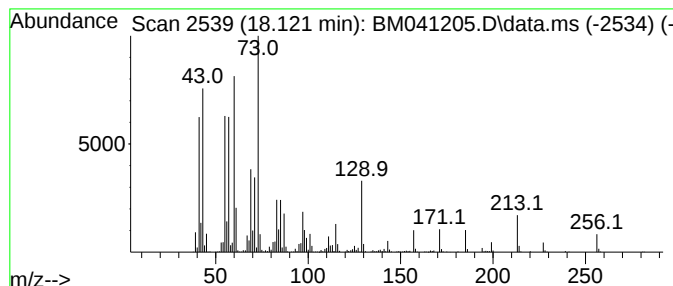
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	10.62 ng	1101380	Phenanthrene-d10	17.221

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	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041205.D
Acq On : 01 Aug 2023 02:05
Operator : MA/JU
Sample : 03741-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P24A

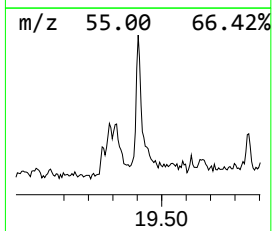
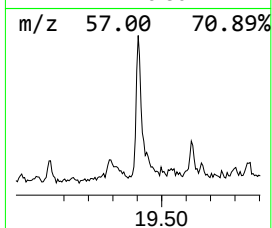
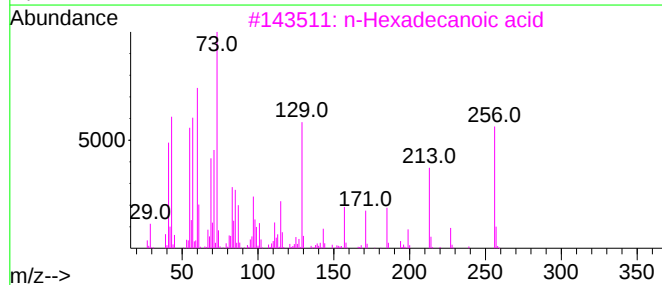
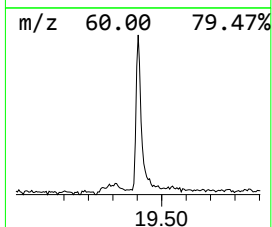
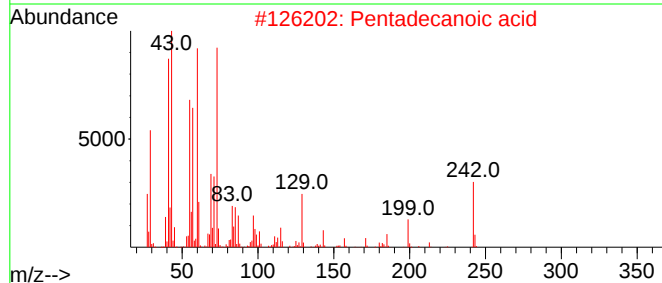
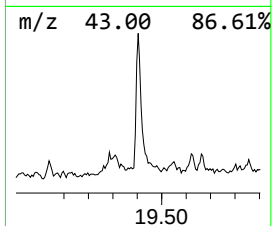
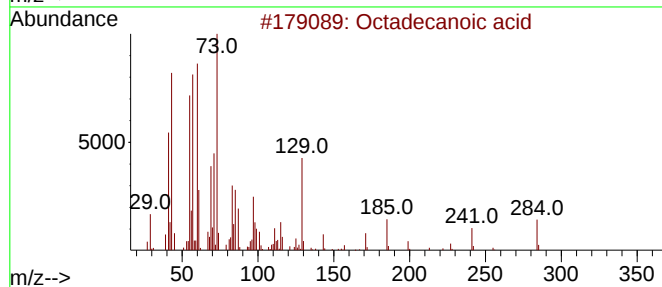
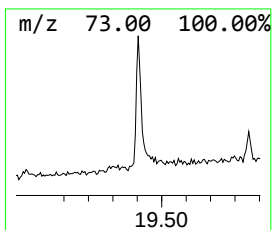
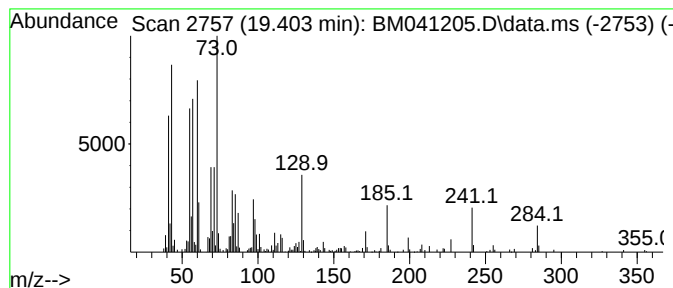
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	2.46 ng	270733	Chrysene-d12	21.421

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	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041205.D
Acq On : 01 Aug 2023 02:05
Operator : MA/JU
Sample : 03741-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P24A

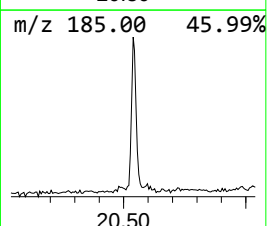
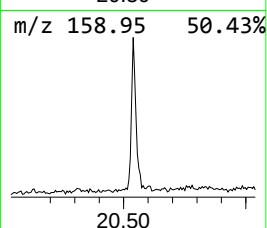
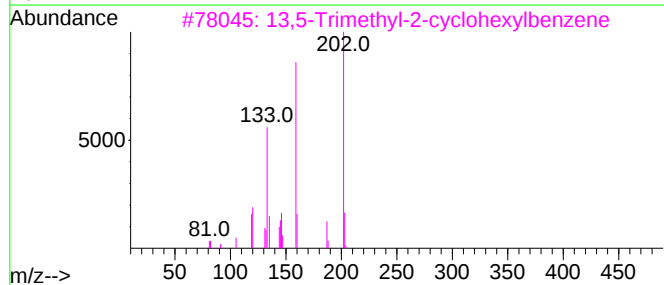
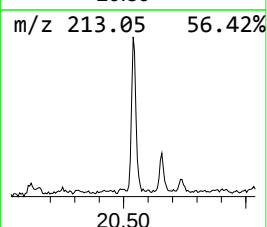
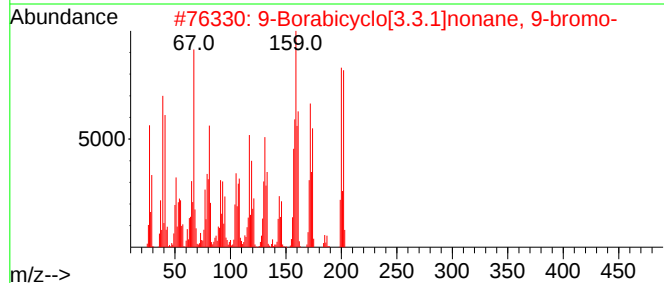
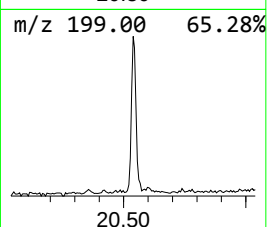
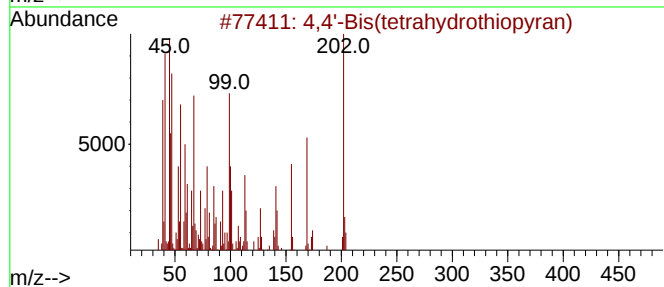
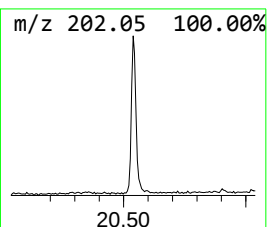
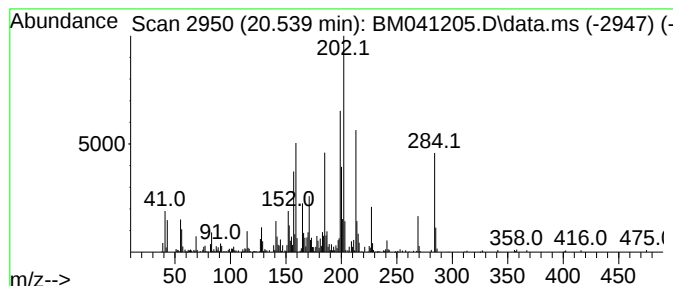
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.539	2.61 ng	286872	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	90
2			9-Borabicyclo[3.3.1]nonane, 9-br...	200	C8H14BBr	022086-45-9	60
3			13,5-Trimethyl-2-cyclohexylbenzene	202	C15H22	004516-10-3	20
4			[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	20
5			4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041205.D
Acq On : 01 Aug 2023 02:05
Operator : MA/JU
Sample : 03741-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P24A

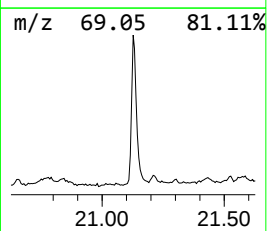
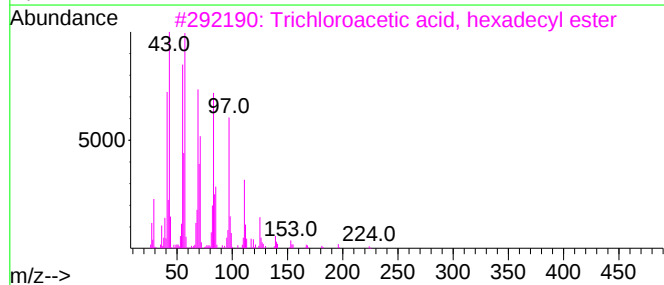
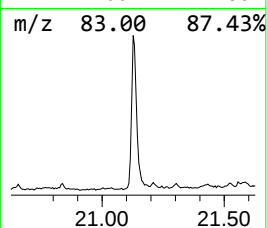
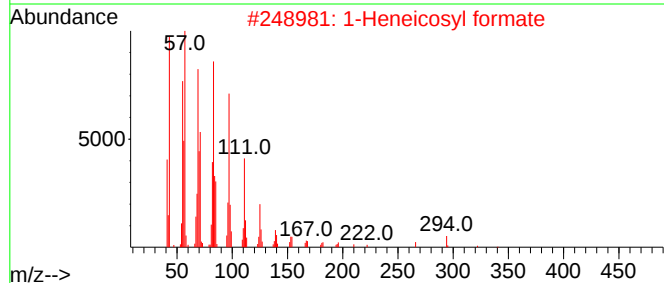
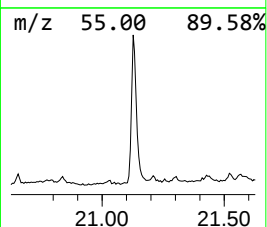
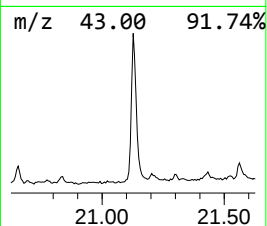
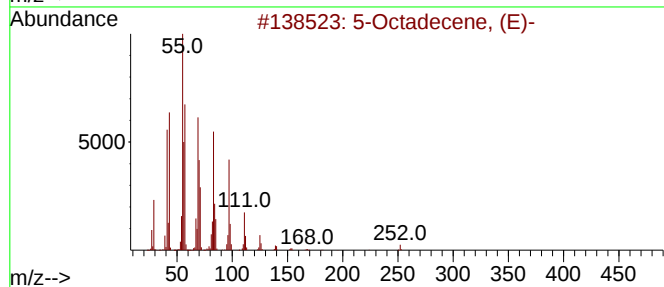
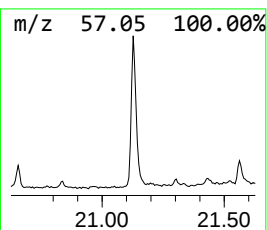
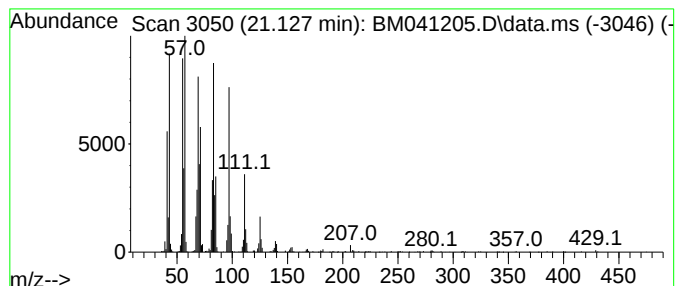
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	7.46 ng	821139	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041205.D
Acq On : 01 Aug 2023 02:05
Operator : MA/JU
Sample : 03741-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P24A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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
Furan, 2,3-dihy...	7.563	2.0	ng	109177	1	7.798	1085080	20.0
2-Cyclohexen-1-one	7.887	5.4	ng	291809	1	7.798	1085080	20.0
Benzaldehyde, 2...	8.316	4.8	ng	262258	1	7.798	1085080	20.0
Catechol	10.410	14.7	ng	1072560	2	10.604	1463460	20.0
Salicyl alcohol	11.645	3.0	ng	220829	2	10.604	1463460	20.0
n-Hexadecanoic ...	18.121	10.6	ng	1101380	4	17.221	2074600	20.0
Octadecanoic acid	19.404	2.5	ng	270733	5	21.421	2202360	20.0
4,4'-Bis(tetrahydro...	20.539	2.6	ng	286872	5	21.421	2202360	20.0
5-Octadecene, (E)-	21.127	7.5	ng	821139	5	21.421	2202360	20.0