

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
 Data File : BG050788.D
 Acq On : 29 Oct 2021 22:06
 Operator : CG/JU
 Sample : M4406-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 280243

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-BG100621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050788.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.780	383	390	403	rBV	608417	1026286	23.76%	7.390%
2	7.389	655	664	673	rBV	617723	1125959	26.06%	8.108%
3	8.241	802	809	823	rVB	131510	238959	5.53%	1.721%
4	9.417	1001	1009	1020	rBV	408547	770637	17.84%	5.549%
5	10.815	1241	1247	1254	rBV	69361	131885	3.05%	0.950%
6	11.068	1284	1290	1299	rVB	186671	357160	8.27%	2.572%
7	12.154	1470	1475	1482	rVB3	73225	156618	3.63%	1.128%
8	13.494	1698	1703	1708	rBV	984525	1570377	36.35%	11.308%
9	14.217	1821	1826	1831	rBV	2915670	4320189	100.00%	31.108%
10	14.628	1891	1896	1900	rBV3	1237333	2734753	63.30%	19.692%
11	22.813	3284	3289	3297	rVB2	520964	920597	21.31%	6.629%
12	25.345	3712	3720	3732	rVB3	163732	534075	12.36%	3.846%

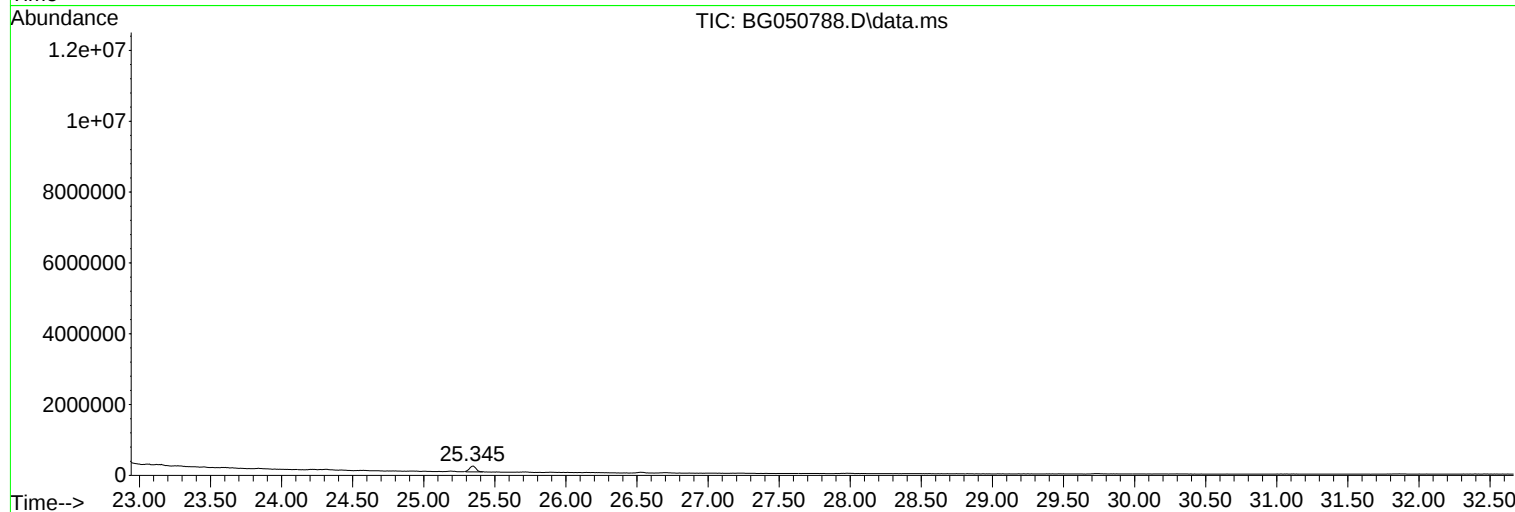
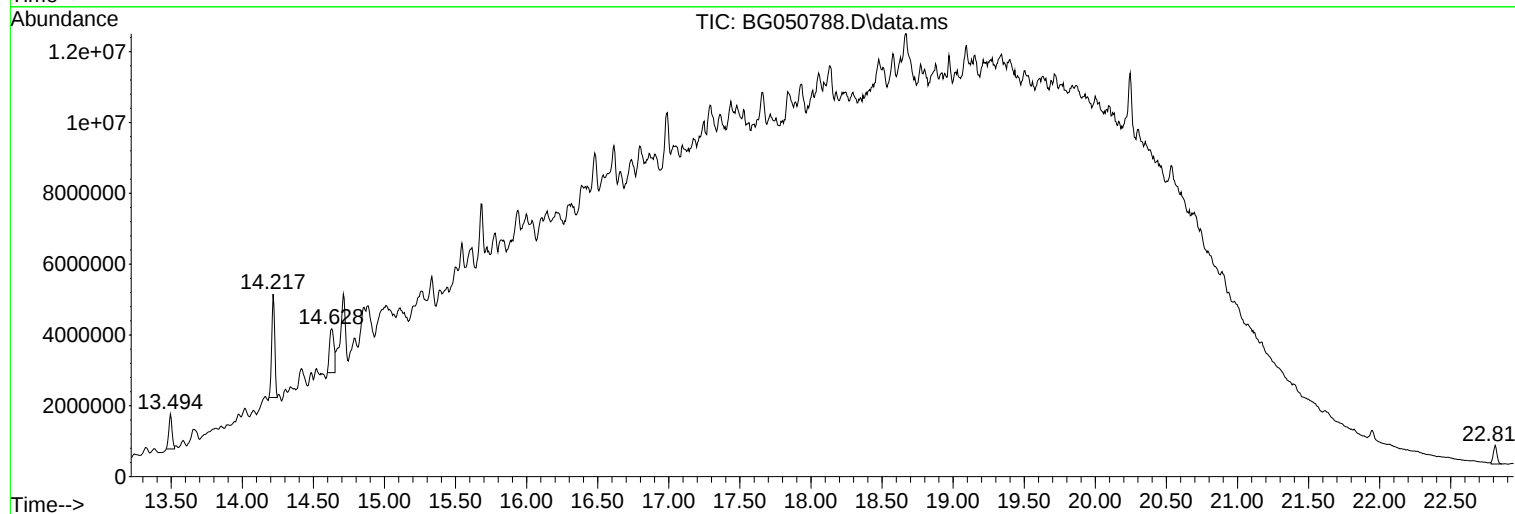
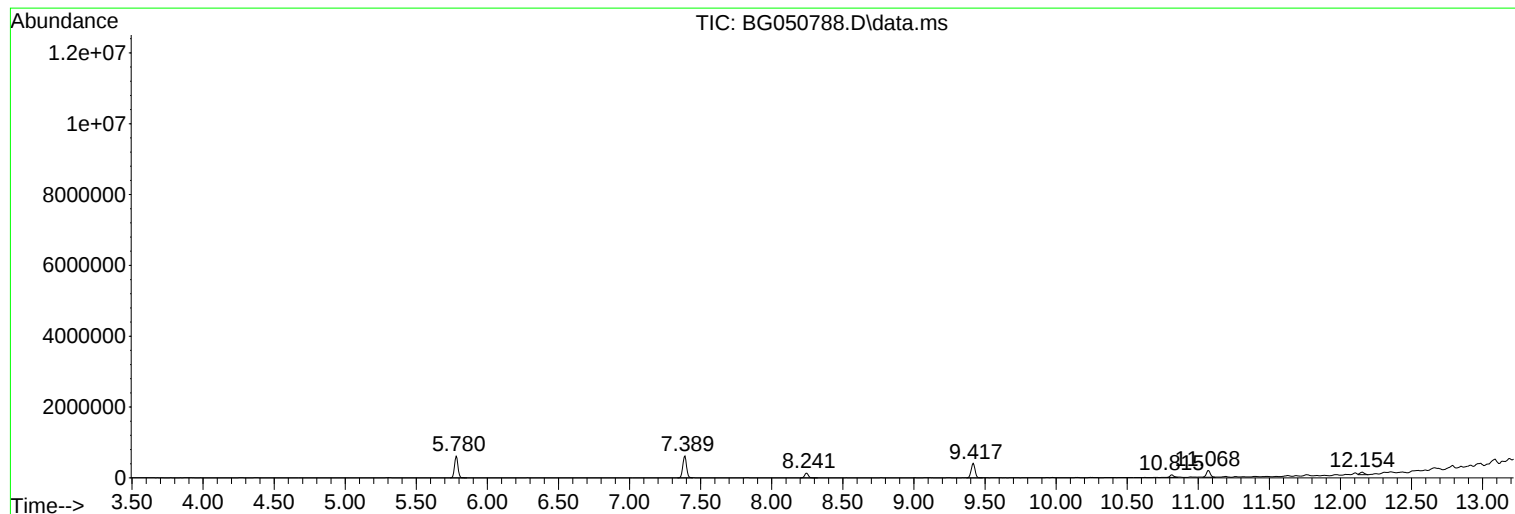
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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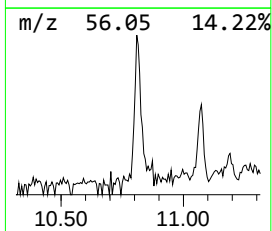
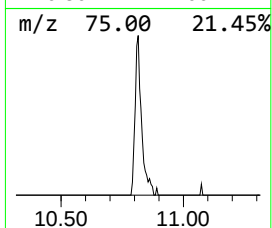
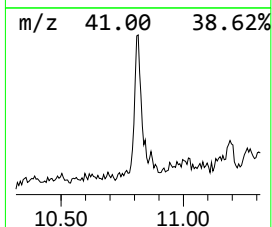
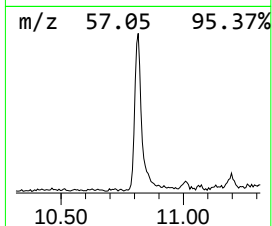
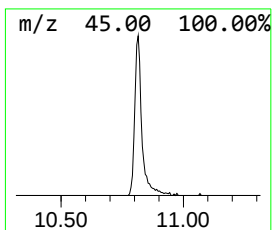
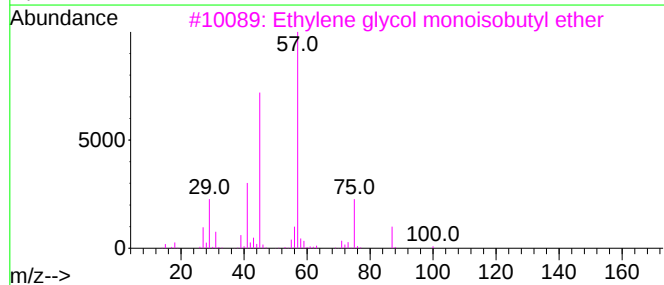
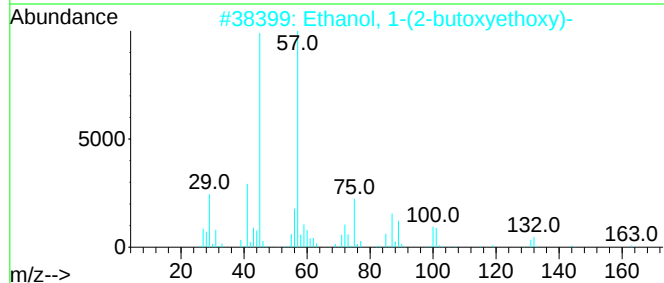
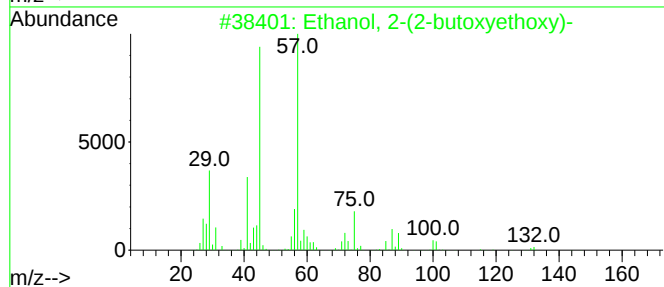
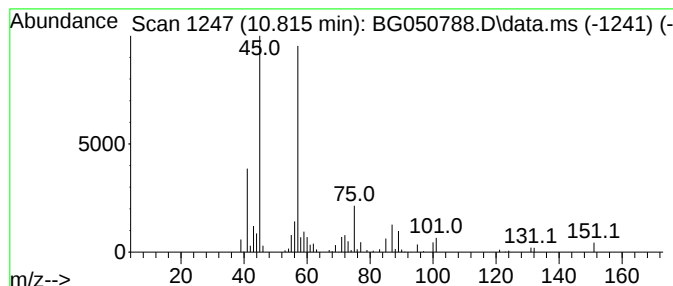
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.815	7.39 ng	131885	Naphthalene-d8	11.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	80
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	47
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	45



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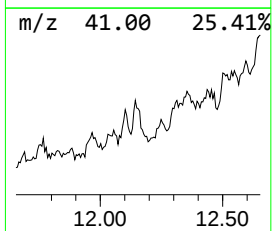
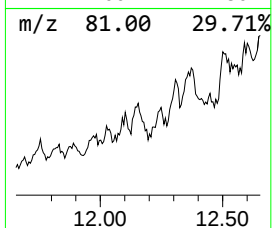
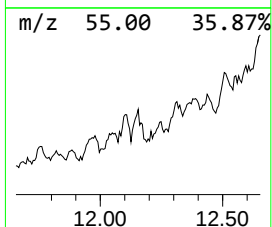
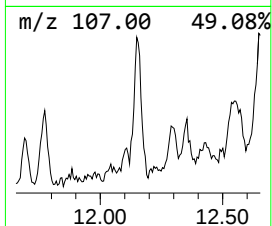
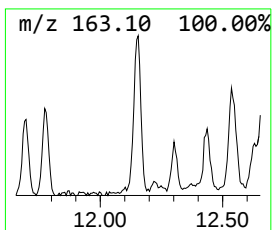
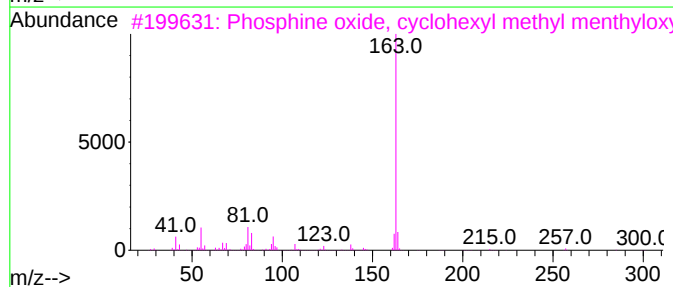
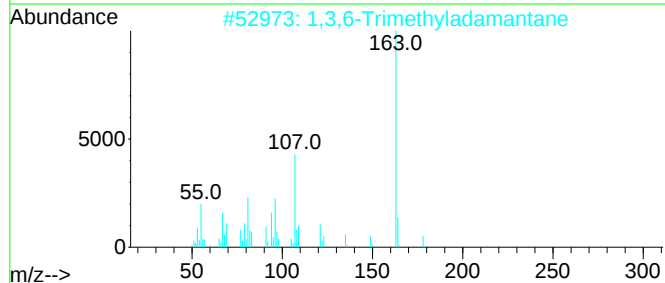
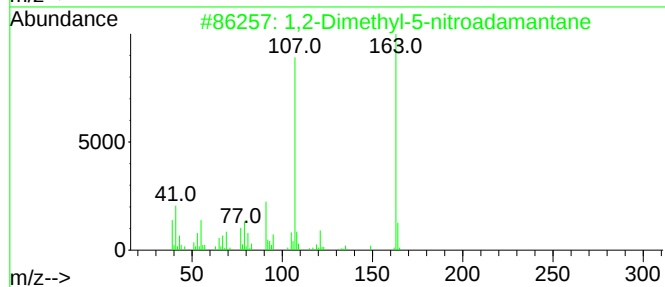
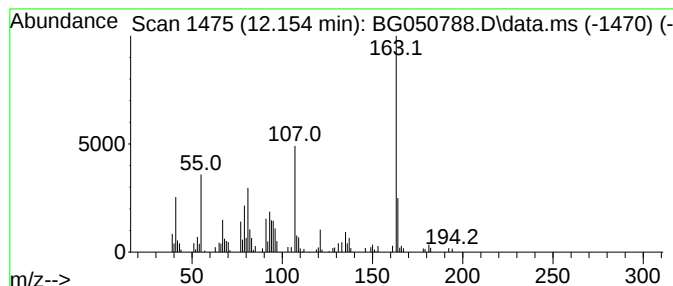
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Peak Number 2 1,2-Dimethyl-5-nitroadamantane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.155	8.77 ng	156618	Naphthalene-d8	11.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	59
2			1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	45
3			Phosphine oxide, cyclohexyl meth...	300	C17H33O2P	1000195-73-8	43
4			1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	42
5			benzoxazole, 7-methoxy-2-methyl-	163	C9H9NO2	1000404-43-8	42



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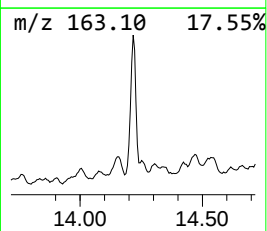
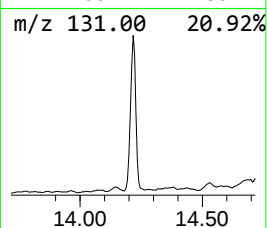
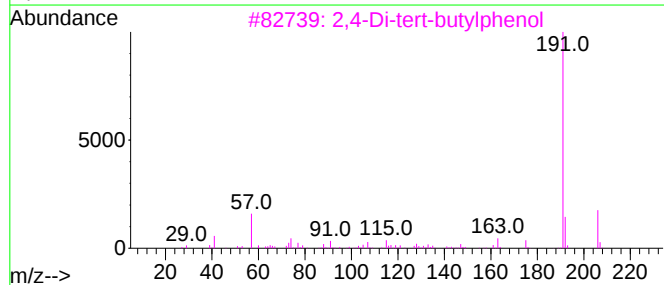
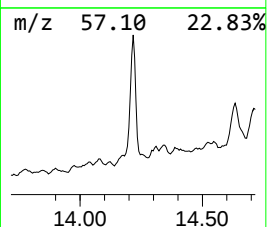
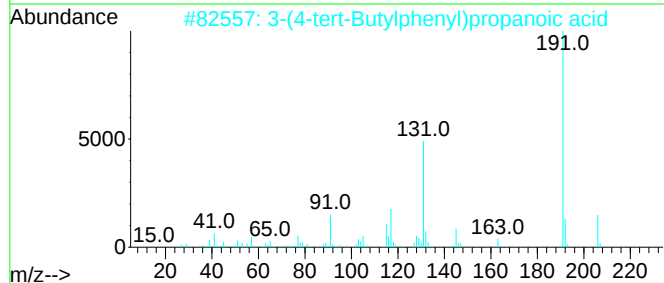
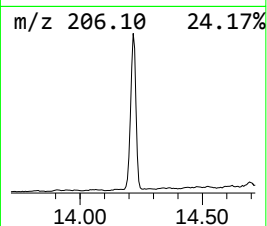
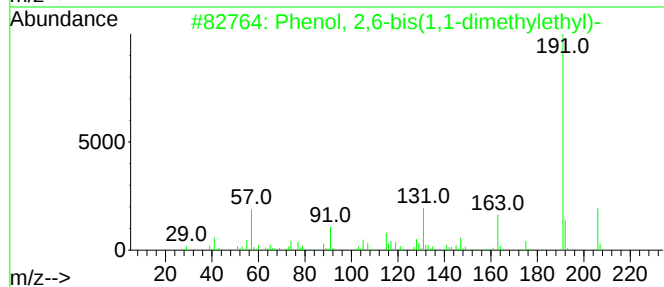
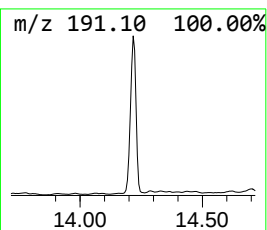
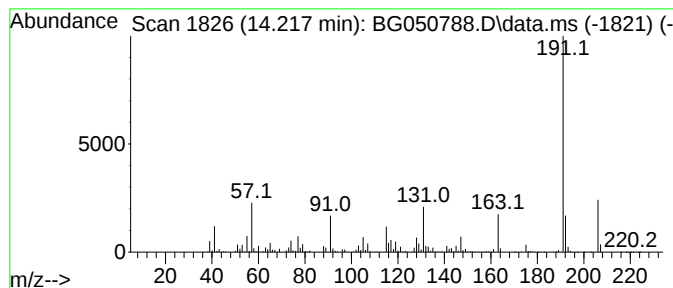
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Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	31.59 ng	4320190	Acenaphthene-d10	14.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	87
3			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	81
4			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	81
5			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	72



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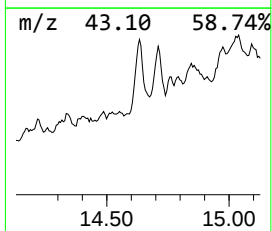
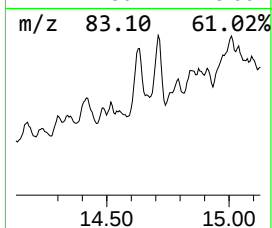
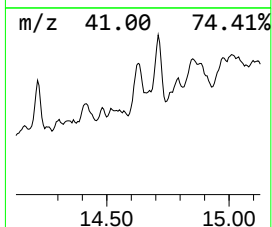
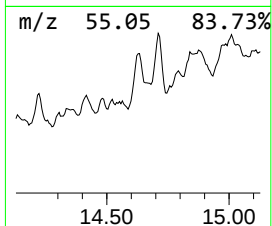
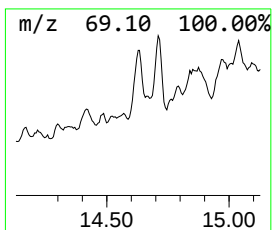
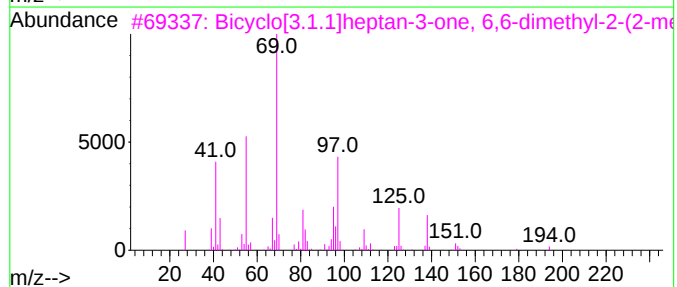
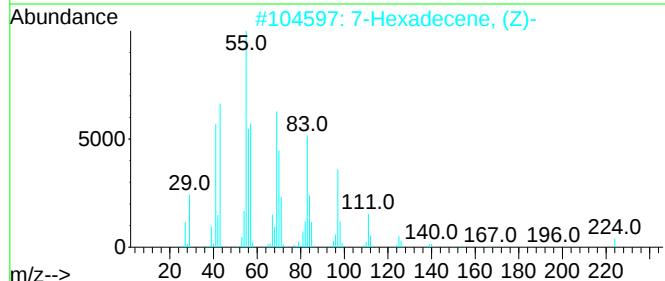
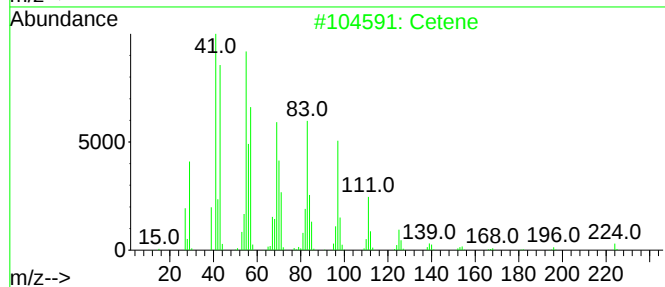
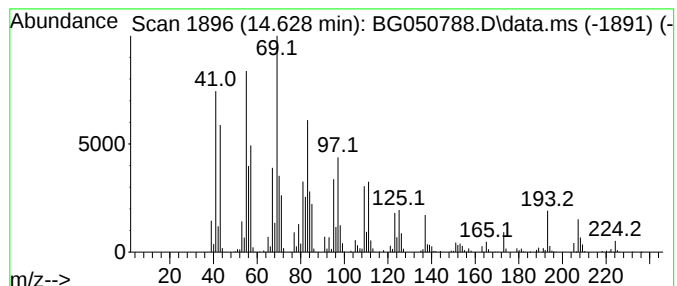
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Peak Number 4 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.628	20.00 ng	2734750	Acenaphthene-d10	14.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	60
2			7-Hexadecene, (Z)-	224	C16H32	035507-09-6	46
3			Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	46
4			1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5	46
5			1-Hexadecanol	242	C16H34O	036653-82-4	45



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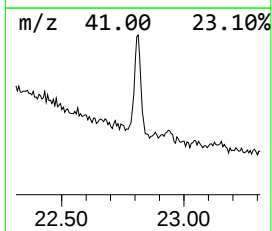
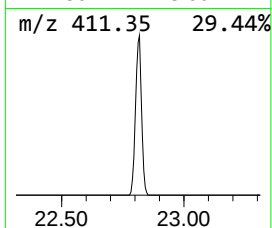
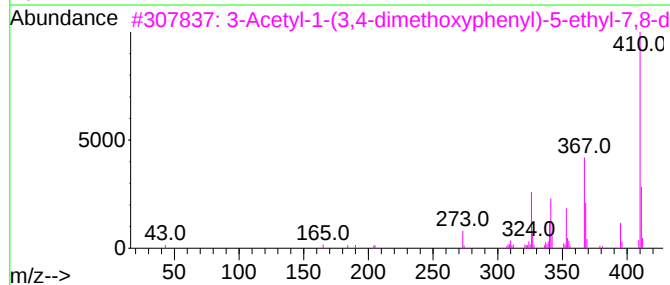
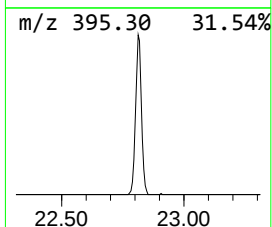
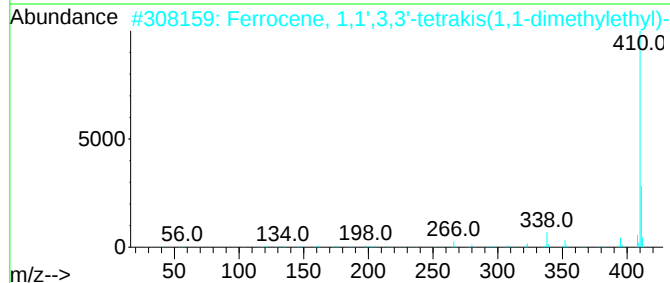
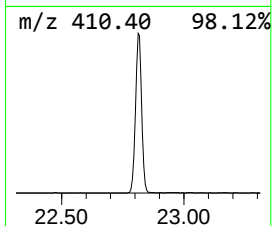
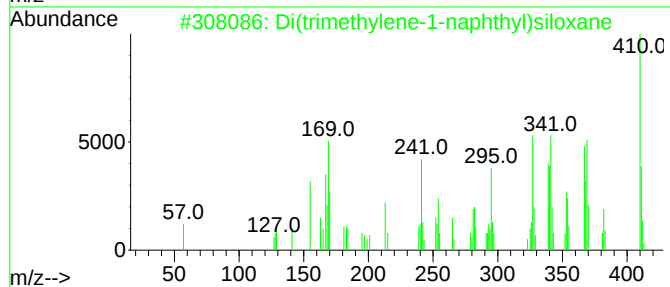
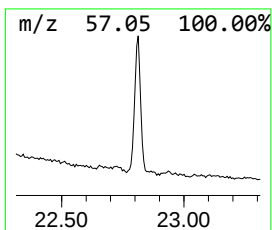
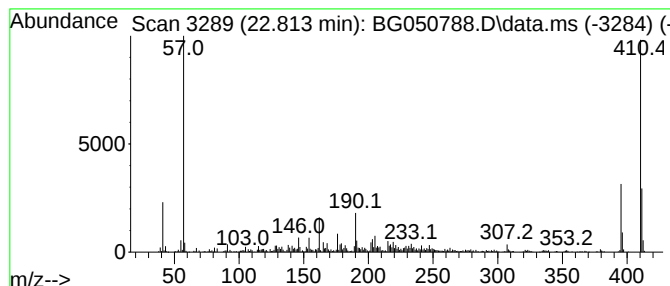
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Peak Number 5 Di(trimethylene-1-naphthyl)... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.813	20.00 ng	920597	Chrysene-d12	21.949

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di(trimethylene-1-naphthyl)siloxane	410	C26H26OSi2	093241-94-2	60
2			Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	58
3			3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	42
4			2-quinoxalinecarbonitrile, 6-(di...	410	C25H38N4O	1000399-06-1	25
5			2'-Hydroxy-3,4,5'-trimethoxychal...	410	C20H17F3O6	1000449-43-5	15



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.815	7.4	ng	131885	2	11.068	357160	20.0
1,2-Dimethyl-5-...	12.155	8.8	ng	156618	2	11.068	357160	20.0
Phenol, 2,6-bis...	14.217	31.6	ng	4320190	3	14.887	2734750	20.0
Cetene	14.628	20.0	ng	2734750	3	14.887	2734750	20.0
Di(trimethylene...	22.813	20.0	ng	920597	5	21.949	920597	20.0