

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
 Data File : BG055960.D
 Acq On : 14 Dec 2022 15:22
 Operator : CG/JU
 Sample : N5993-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AOC1-E5

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055960.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.406	15	20	25	rBV	22850	31177	4.29%	1.276%
2	5.415	357	362	367	rBB	11259	16931	2.33%	0.693%
3	5.885	436	442	448	rBB	80983	126571	17.41%	5.181%
4	7.495	709	716	722	rBB	83337	141355	19.44%	5.786%
5	8.371	859	865	871	rBB	19997	29976	4.12%	1.227%
6	9.540	1057	1064	1071	rBB	47652	81236	11.17%	3.325%
7	11.203	1341	1347	1354	rBB	25414	42670	5.87%	1.747%
8	13.606	1750	1756	1763	rBB	187085	289877	39.87%	11.866%
9	14.975	1984	1989	1995	rBB	49568	77681	10.68%	3.180%
10	16.314	2212	2217	2222	rBB	15684	20884	2.87%	0.855%
11	16.450	2234	2240	2247	rBV	226707	351551	48.35%	14.390%
12	17.713	2448	2455	2462	rBV	86685	124899	17.18%	5.113%
13	20.292	2888	2894	2899	rBV	552860	727101	100.00%	29.763%
14	20.386	2904	2910	2918	rVV6	4862	13269	1.82%	0.543%
15	21.614	3111	3119	3128	rVB6	13091	27015	3.72%	1.106%
16	22.019	3181	3188	3196	rBV2	99285	162998	22.42%	6.672%
17	25.509	3770	3782	3795	rBV2	59477	177776	24.45%	7.277%

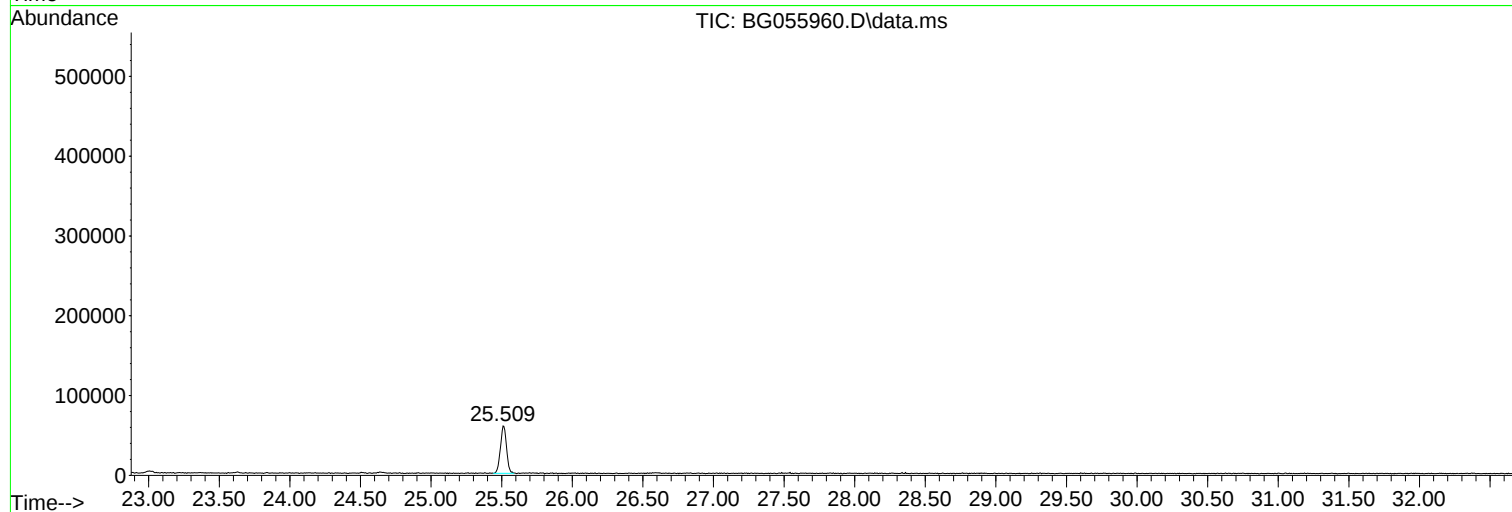
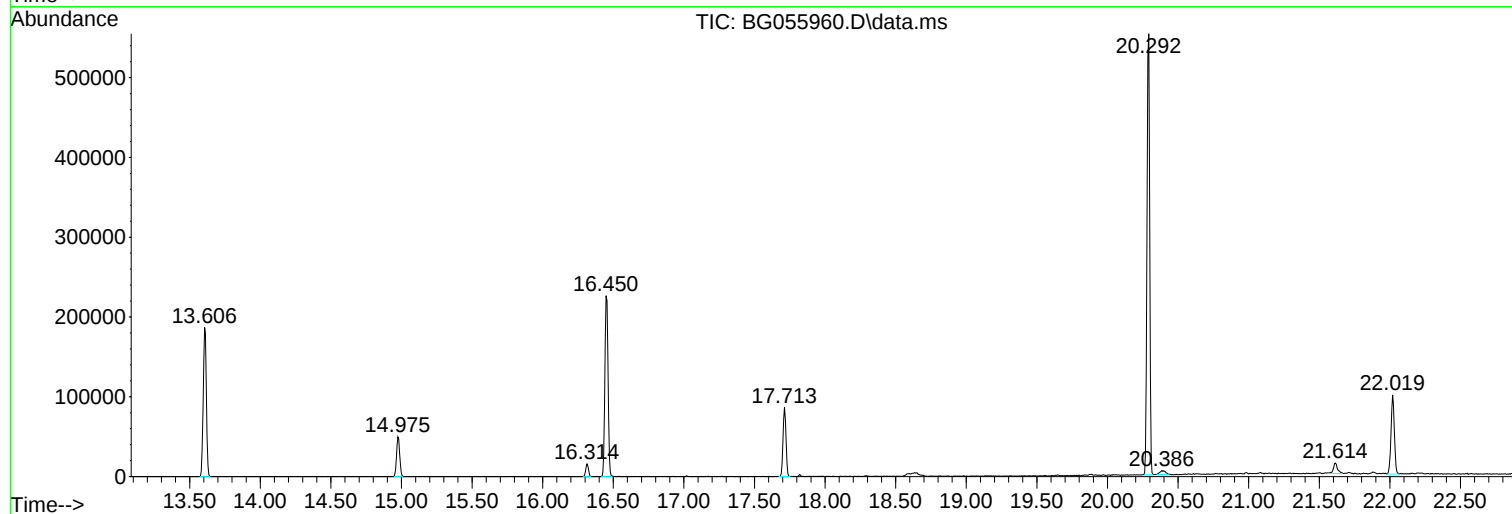
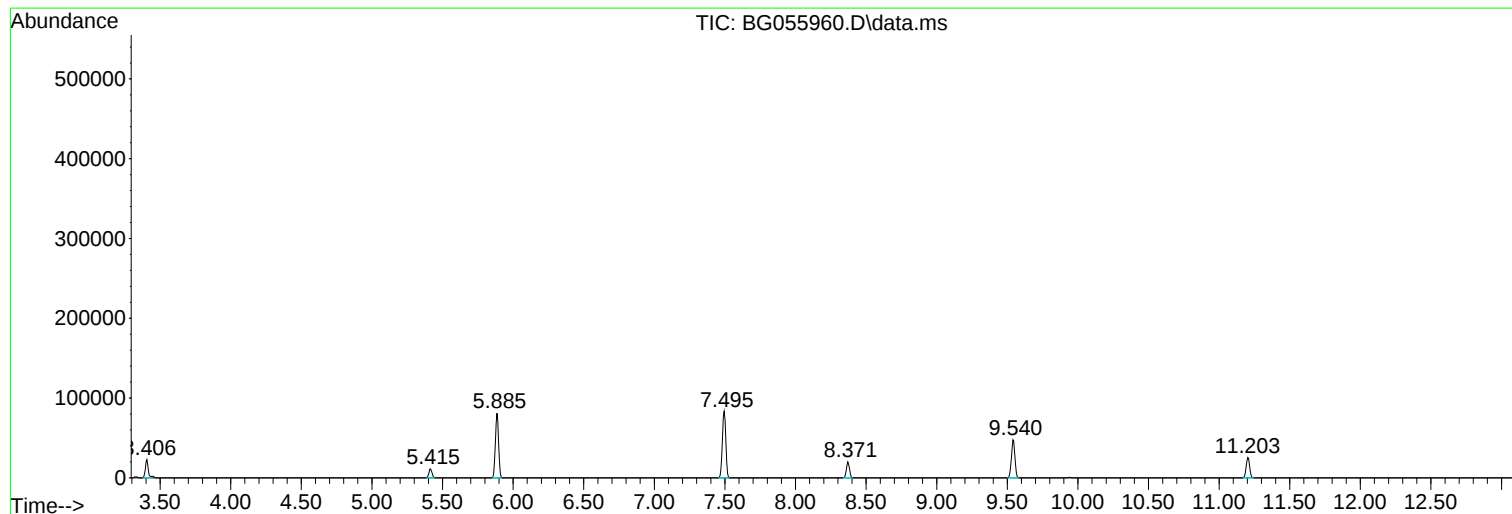
Sum of corrected areas: 2442967

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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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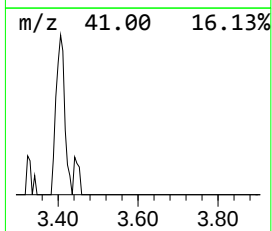
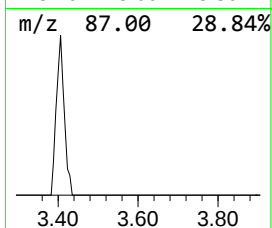
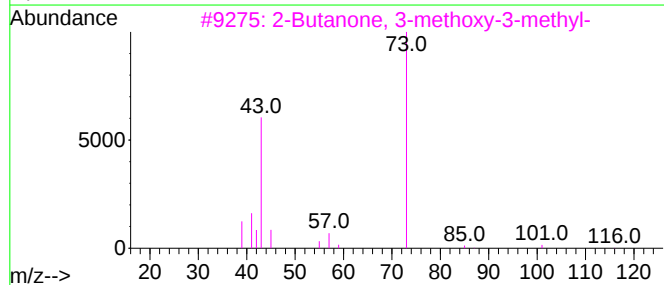
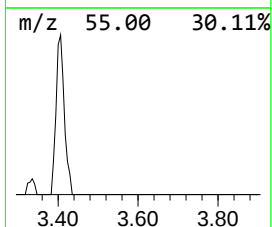
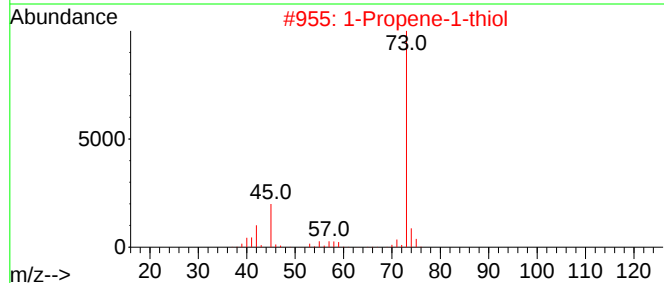
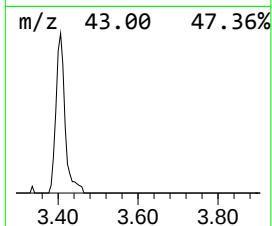
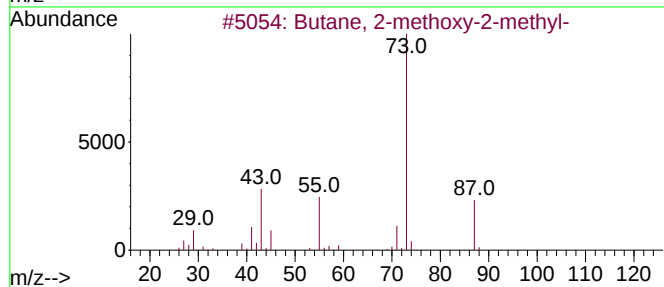
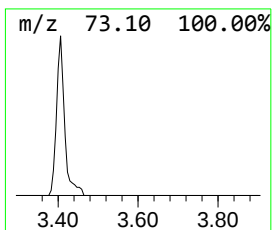
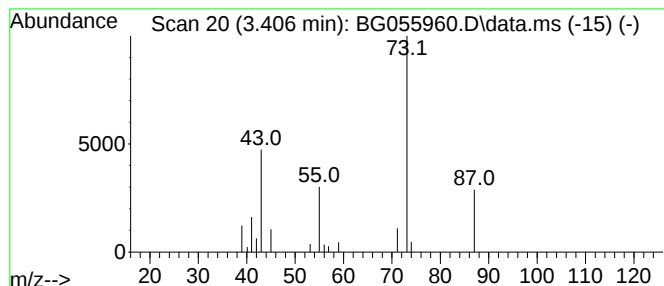
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.406	20.80 ng	31177	1,4-Dichlorobenzene-d4	8.371

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
3			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9



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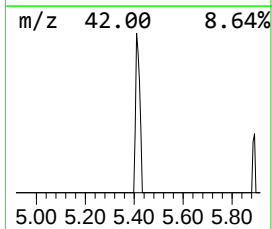
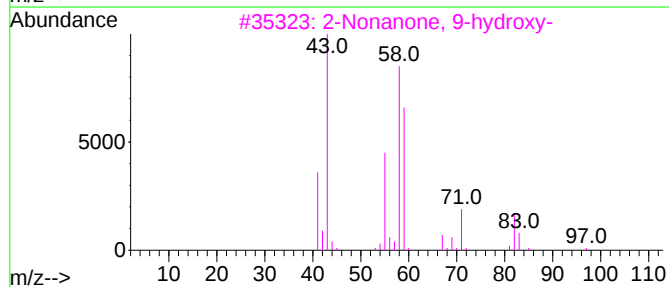
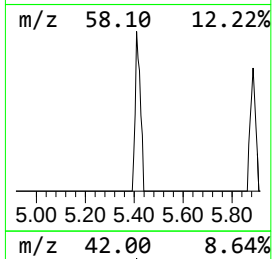
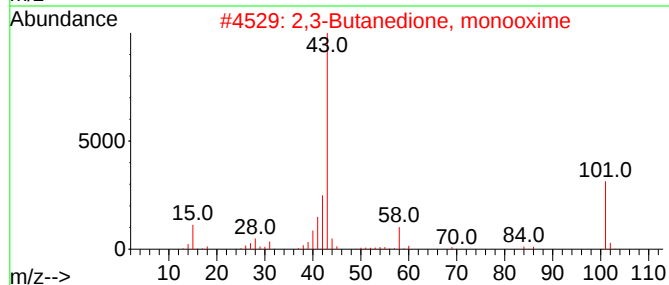
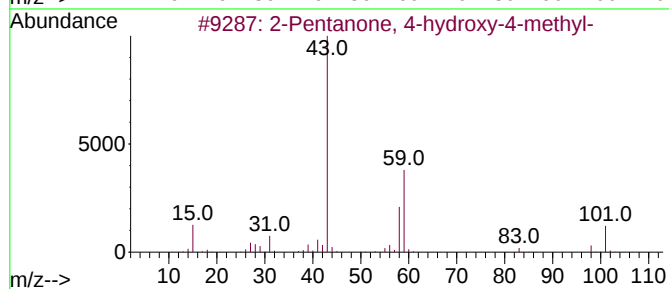
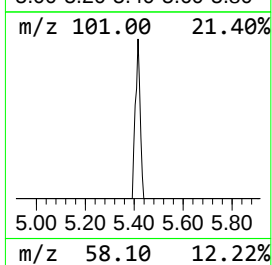
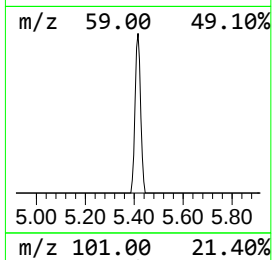
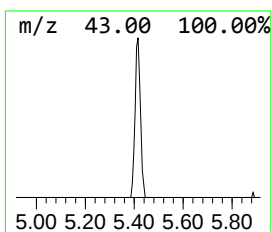
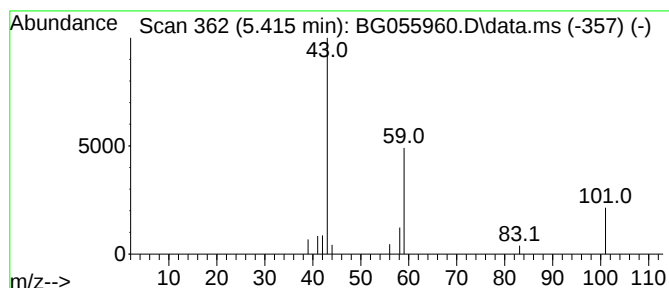
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.415	11.30 ng	16931	1,4-Dichlorobenzene-d4	8.371

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9
4			Propylamine	59	C3H9N	000107-10-8	7
5			Butane	58	C4H10	000106-97-8	7



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ALS Vial : 5 Sample Multiplier: 1

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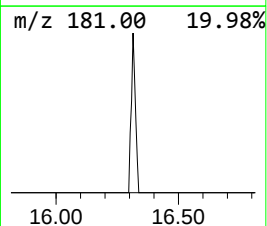
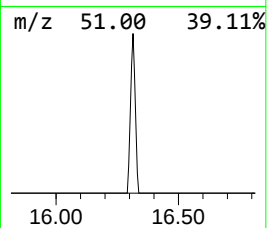
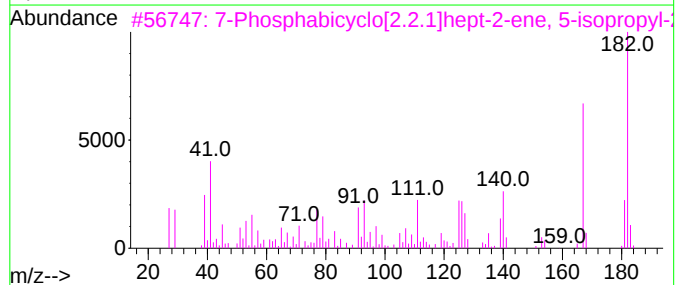
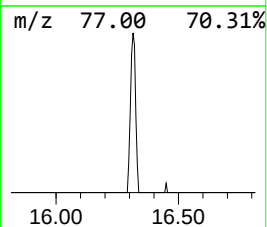
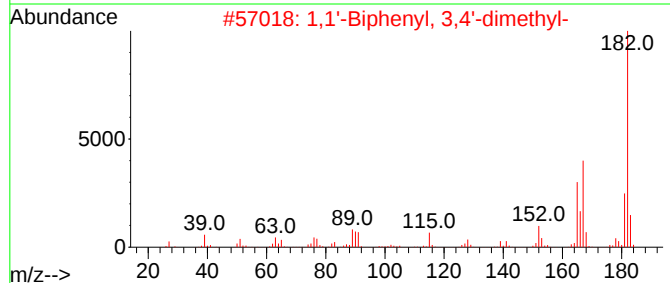
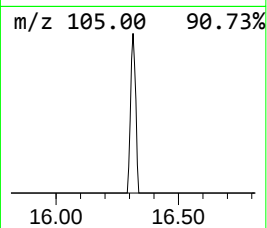
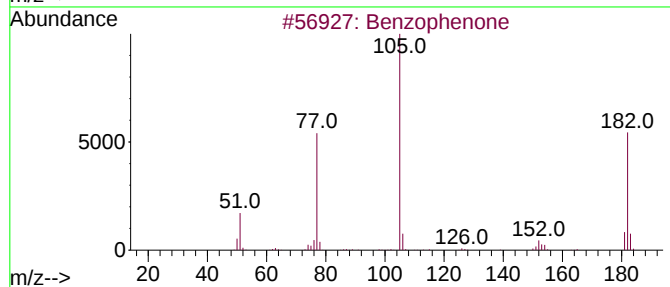
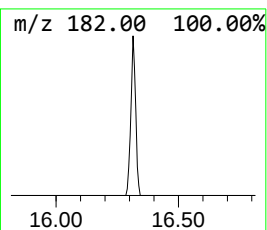
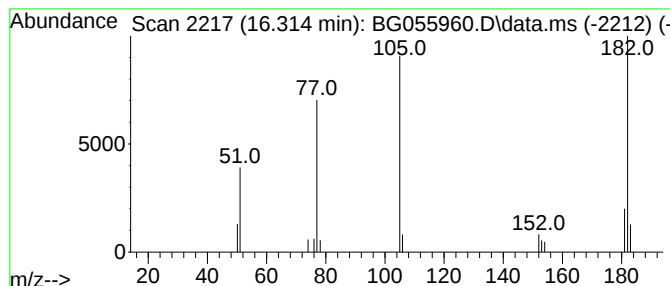
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.314	5.38 ng	20884	Acenaphthene-d10	14.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	43
3			7-Phosphabicyclo[2.2.1]hept-2-en...	182	C11H19P	1000151-83-5	38
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	38
5			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	38



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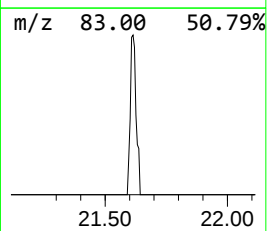
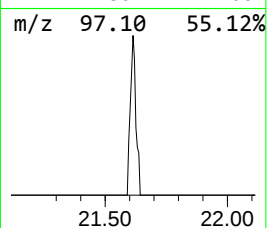
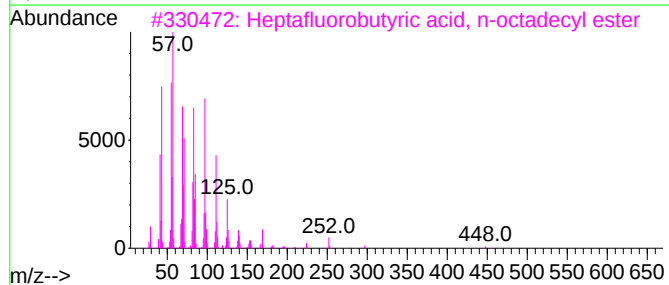
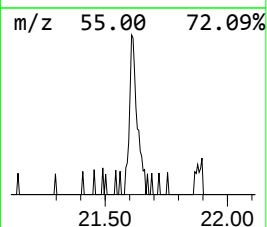
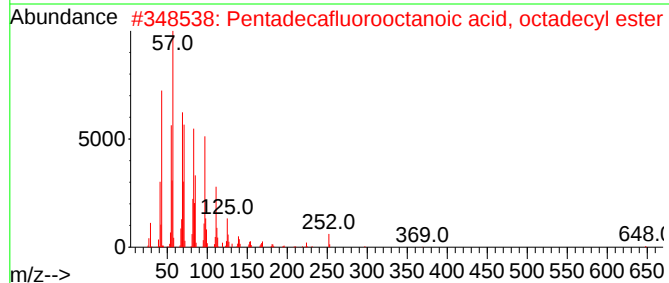
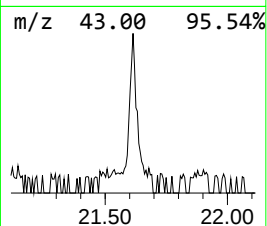
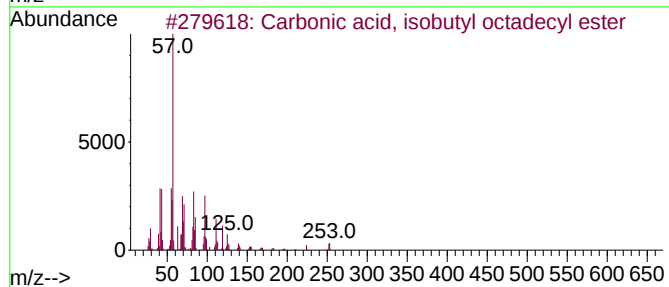
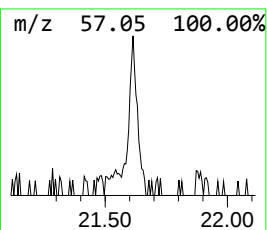
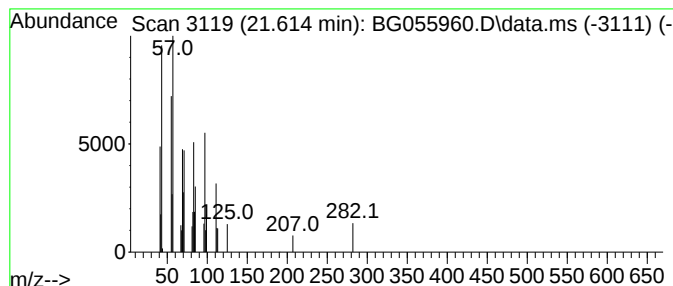
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Peak Number 4 Carbonic acid, isobutyl oct... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.614	3.31 ng	27015	Chrysene-d12	22.020

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
3			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87
4			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	87
5			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.406	20.8	ng	31177	1	8.371	29976	20.0
2-Pentanone, 4-...	5.415	11.3	ng	16931	1	8.371	29976	20.0
Benzophenone	16.314	5.4	ng	20884	3	14.975	77681	20.0
Carbonic acid, ...	21.614	3.3	ng	27015	5	22.020	162998	20.0